



A Microscopic Theory of Fission (part I)

FIESTA 2014 Summer School

W. Younes

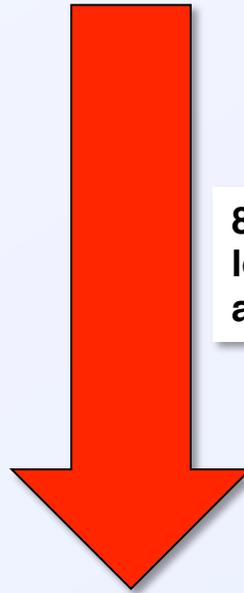
Physical and
Life Sciences

Lawrence Livermore National Laboratory

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"it is conceivable that the nucleus breaks up into several large fragments, which would of course be isotopes of known elements but would not be neighbors of the irradiated element." – Ida Noddak (1934)



80 years later, there is still a lot we don't understand about fission!

"Problems worthy of attack prove their worth by hitting back" – Piet Hein



A complex problem that has spawned different lines of attack

Liquid-drop model (1939-) + shell corrections

J. Randrup and P. Möller,
Phys. Rev. Lett. 106, 132503 (2011)

Statistical scission-point models (1970's-)

S. Panebianco et al.,
Phys. Rev. C 86, 064601 (2012)

Microscopic models (1980's-)

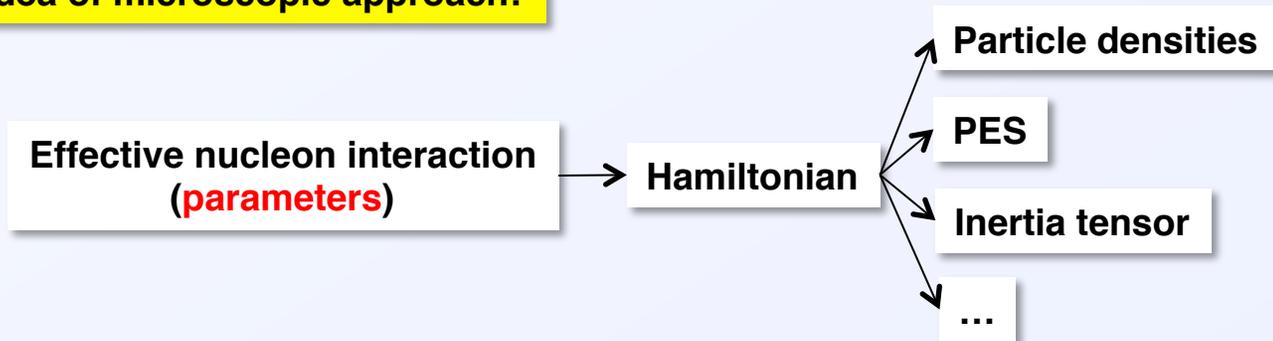
- Fragment yields
- Fragment kinetic energies
- Fragment excitation energies
- Fission probabilities
- Fission cross sections
- Fission times
- Scission neutrons
- ...

All these approaches (and others) bring valuable insights into what is arguably the most challenging problem in nuclear physics



What is the microscopic approach?

Idea of microscopic approach:



Effective interaction is the only phenomenological input

The hierarchy of the microscopic approach

- Starting point is effective interaction between nucleons
 - Finite-range, fit a-priori, to very few nuclear data
- Simplest treatment of nucleon correlations is Mean Field
 - Valid if nearby excitations \gg residual interaction (e.g., magic nuclei)
 - Otherwise true wave function mixes with nearby excitations
- Introduce correlations into Hamiltonian via successive improvements
 1. $H_{\text{true}} \approx H_{\text{MF}}$ (Hartree-Fock)
 2. $H_{\text{true}} \approx H_{\text{MF}} + V_{\text{pair}}$ (Hartree-Fock-Bogoliubov)
 3. $H_{\text{true}} \approx H_{\text{MF}} + V_{\text{pair}} + V_{\text{coll}}$ (Generator-coordinate method)
 4. $H_{\text{true}} \approx H_{\text{MF}} + V_{\text{pair}} + V_{\text{coll}} + V_{\text{coll-intr}}$ (GCM + qp excitations)
 5. ...

Tractable approach to a microscopic treatment of fission



Features of the microscopic approach useful for fission

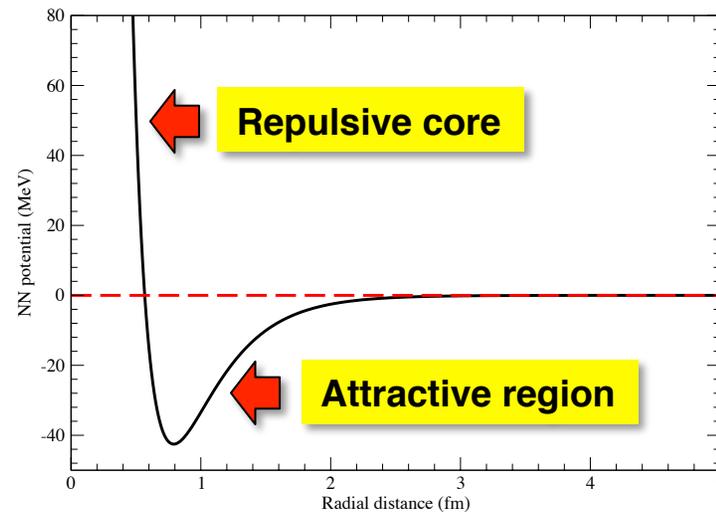
- **Ingredients: protons, neutrons, and an effective interaction between them**
- **The spatial distribution of nucleons is a result, not an input**
 - Found by minimizing the energy
 - In a fully microscopic approach, no parameters depending on A , Z , or the configuration of the nucleus
 - Important in fission since the system explores very exotic “shapes”
- **Unified description of both single-particle and collective dof**
 - Mean field constructed from nucleon dof
 - Residual interactions between nucleons can then cause this mean field to oscillate , generating a spectrum of collective states
- **Starting point is Hamiltonian of A interacting nucleons**
 - Quantum mechanics is built in from the start

But there are major challenges...



Challenge 1: we don't have a fundamental theory of the nucleon-nucleon interaction

We do not yet have a nuclear interaction completely derived from QCD



Although important progress is being made in that direction
(see, e.g., http://www.cenbg.in2p3.fr/heberge/EcoleJoliotCurie/coursannee/cours/D_lacroix.pdf)

For now, we use an effective interaction, with parameters adjusted to data

Where do effective interactions come from?

- Realistic NN interactions cannot be used directly in many-body calculations because repulsive core prevents perturbative approach
- Brueckner & Goldstone devised a way to carry out the sums of infinite numbers of terms that account for the two-body interactions
- Inside the nuclear medium, Pauli exclusion limits the number of states that two nucleons can scatter into and prevents divergences due to the core
 - Thus the problematic bare interaction is replaced by a well-behaved “G matrix” describing the scattering of two nucleons inside the medium
 - The G matrix is the most important example of an effective interaction for the nucleus
 - Inside infinite nuclear matter, the Brueckner-Goldstone prescription can be calculated numerically and guides both the form and parameter values for the phenomenological effective interactions that are commonly used



Effective interactions 101

- The N-N interaction is modified by its presence inside a nucleus
- Can be approximated by simple functional forms
 - Delta function \Rightarrow zero range

T.H.R. Skyrme, Phil. Mag. 1, 1043 (1956)

$$V(\vec{r}_1, \vec{r}_2) \sim \delta(\vec{r}_1 - \vec{r}_2)$$

- Gaussian \Rightarrow finite range

D. Gogny, in “Nuclear self-consistent fields”, p. 333 (1975)

$$V(\vec{r}_1, \vec{r}_2) \sim e^{-(\vec{r}_1 - \vec{r}_2)^2 / \mu^2}$$

- More computationally demanding than delta
- Avoids mathematical pathologies of delta
- This is what I will use for the rest of this lecture

For simplicity, I have not written all the terms.
There are a dozen free parameters from those terms



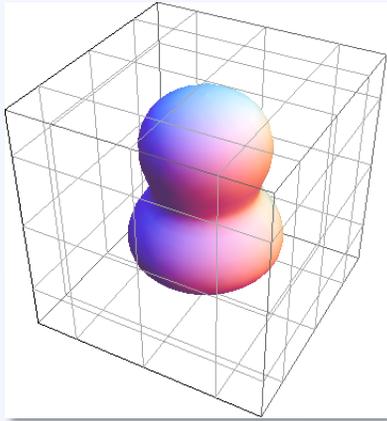
Fixing the parameters of the interaction

- Parameters adjusted to a small number of quantities
 - Infinite nuclear matter
 - Saturation properties (E/A and k_F)
 - Incompressibility K_∞
 - Asymmetry parameter
 - Semi-infinite nuclear matter
 - Surface coefficient
 - Finite nuclei
 - Binding energies of ^{18}O and ^{90}Zr
 - Energy difference $1p_{1/2} - 1p_{3/2}$ in ^{16}O
 - Odd-even mass differences in a few Sn isotopes
 - Barrier height in ^{240}Pu

Important: not tuned to fission observables!



Challenge 2: Fission is a difficult quantum many body problem

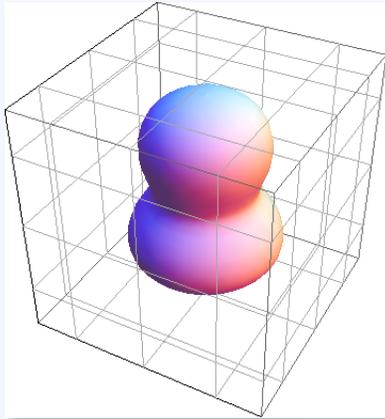


Sizing up the problem with a simplistic calculation:

For ^{240}Pu fission: distribute 94 protons & 146 neutrons on 3D spatial lattice + spin, 20 fm to the side, 1 fm spacing $\Rightarrow 20^3 \times 2 = 16000$ lattice points:

$$\binom{16000}{94} \times \binom{16000}{146} \approx 10^{608} \text{ configurations!!!}$$

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- **Too complicated to describe with full many-body wave function**
- ⇒ **Start with simplified picture, restore complexity in order of importance**
- ⇒ **Need High Performance Computing**
- ⇒ **Need to solve some tough conceptual problems**
 - **What are the relevant degrees of freedom? (collective vs. intrinsic)**
 - **How does the coupling between them affect fission?**
 - **What is scission? How do we separate pre- and post-scission?**
 - ...

The Hartree-Fock approximation

- The full many-body wave function has too many terms

$$\Psi = \sum_{\text{all configs}} c_{\text{config}} |\text{config}\rangle \quad \text{number of terms} \sim \binom{\text{states}}{\text{nucleons}}$$

- There are two commonly used solutions

- The shell model: reduce the number of terms by restricting the number of states and nucleons to a few outside a closed shell
- The Hartree-Fock approximation: replace Ψ with a simpler form:
 - Single Slater determinant, choose the one that minimizes the energy
 - e.g., for a system of 2 nucleons:

$$\Psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \begin{bmatrix} \varphi_a(\vec{r}_1) & \varphi_a(\vec{r}_2) \\ \varphi_b(\vec{r}_1) & \varphi_b(\vec{r}_2) \end{bmatrix} = \frac{1}{\sqrt{2}} [\varphi_a(\vec{r}_1)\varphi_b(\vec{r}_2) - \varphi_b(\vec{r}_1)\varphi_a(\vec{r}_2)]$$

This is not the most general form for $\Psi(1,2,\dots)$: we are sacrificing some particle correlations for the sake of tractability



Solving the Hartree-Fock equations

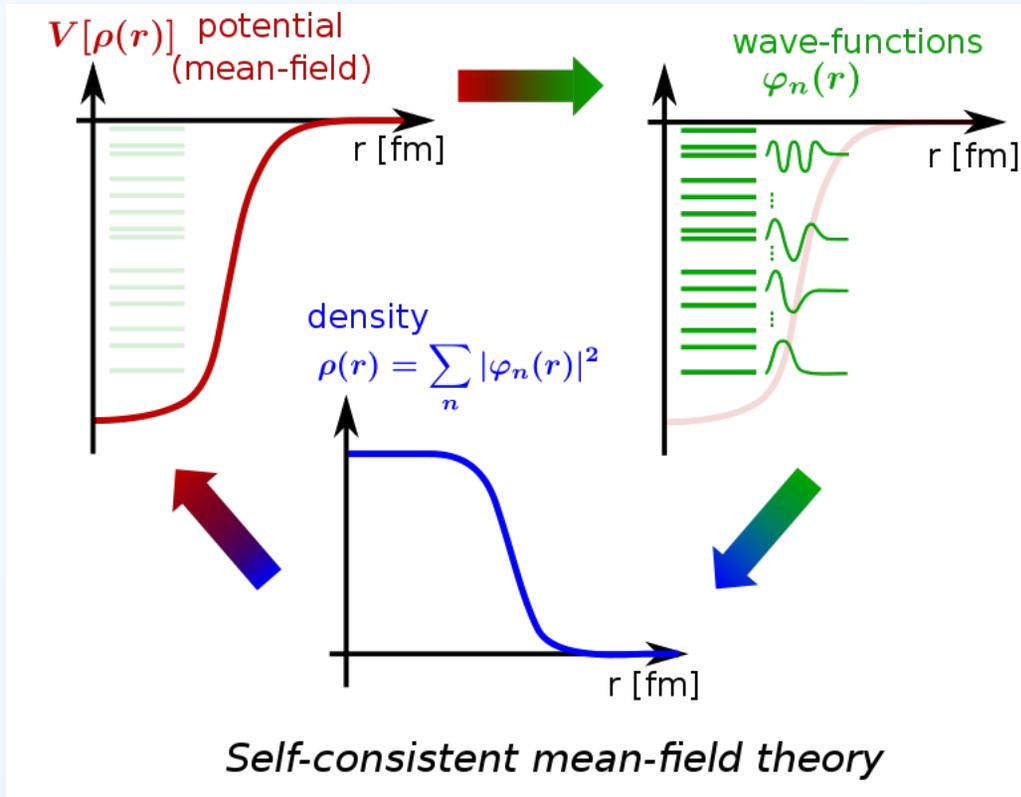
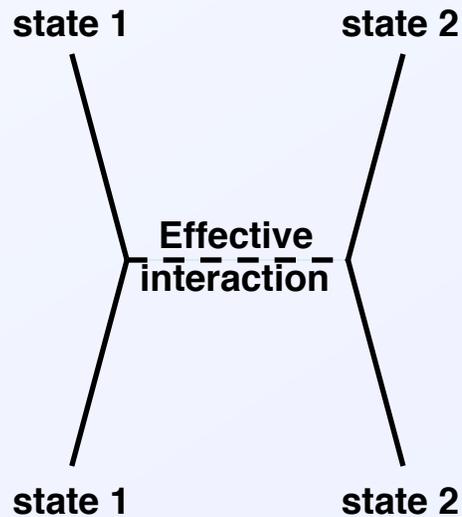


Image from commons.wikimedia.org

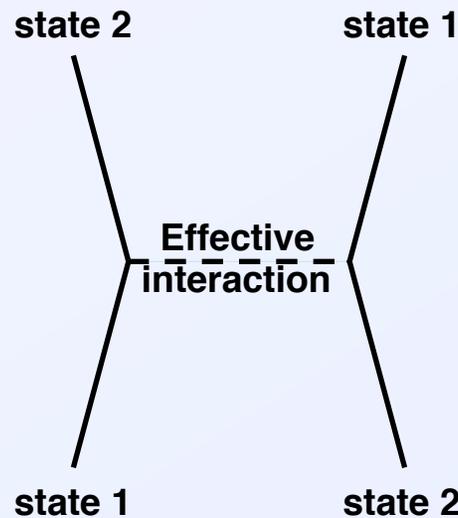
- From the Slater determinant, we calculate a one-particle density ρ
- From ρ we calculate a potential energy
- From the potential energy we get single-particle states $\varphi_n \Rightarrow$ Slater determinant
- \Rightarrow Hartree-Fock eqs are derived by a variational method and solved by an iterative process
- \Rightarrow Independent particles in a mean field, system in its lowest-energy state

Important aspects of the energy calculation

$$\text{mean-field energy} = \sum_{\text{state 1}} \sum_{\text{state 2}}$$

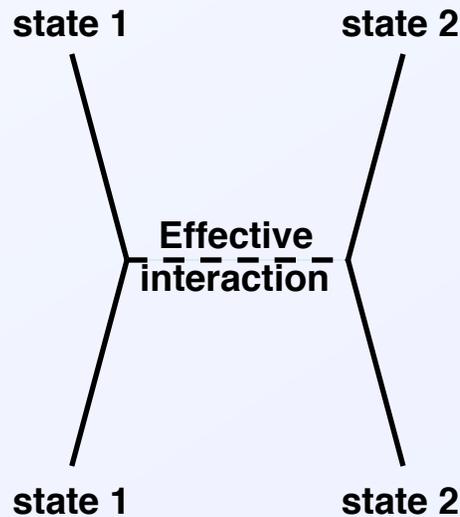


Also includes exchange terms:



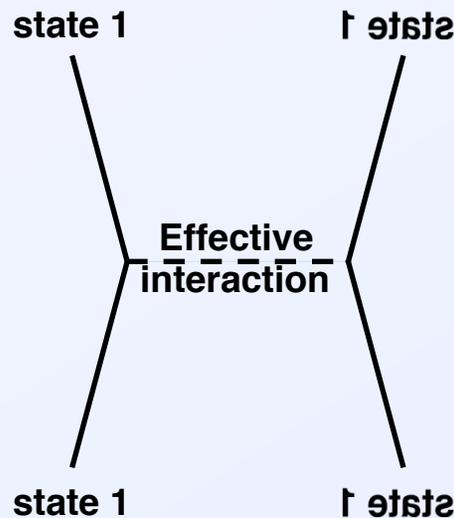
Important aspects of the energy calculation

$$\text{mean-field energy} = \sum_{\text{state 1}} \sum_{\text{state 2}}$$



Also includes pairing:

$$\text{pairing energy} = \sum_{\text{state 1}} \sum_{\text{state 2}}$$

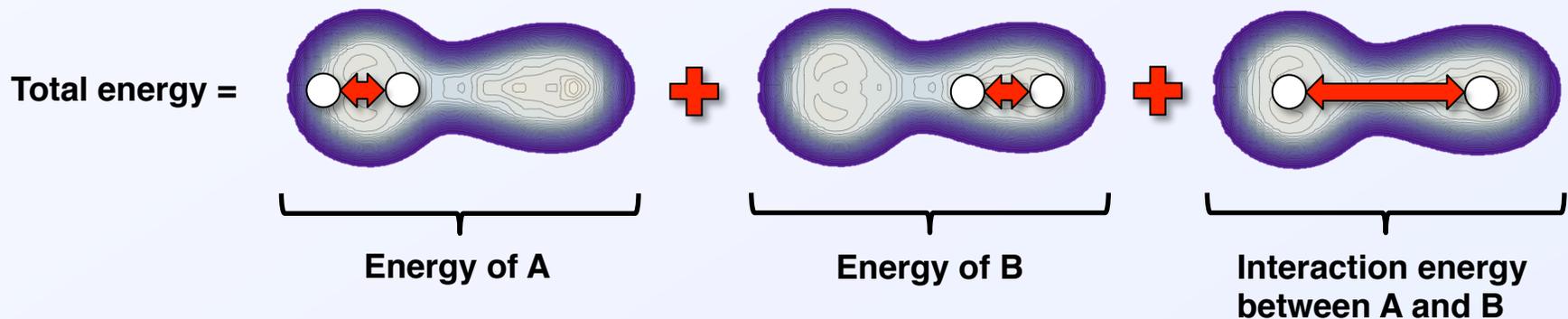


Mean field and pairing involve different states, but the same effective interaction



Important aspects of the energy calculation

- The energy sum extends over all states in the nucleus
- But if you want to distinguish parts of that nucleus, you can always rearrange the terms in the sum:

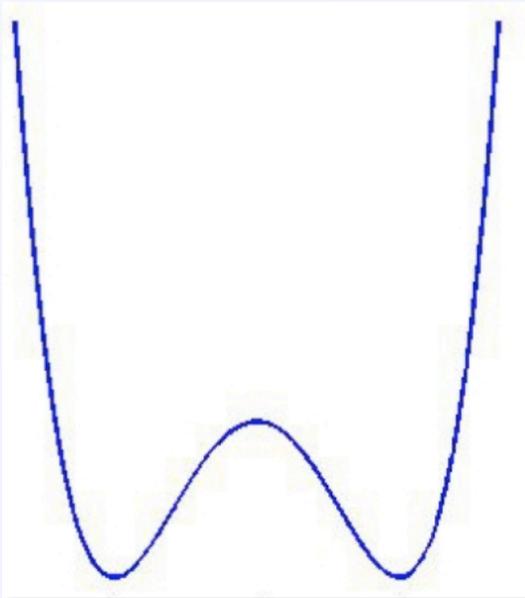


- The same effective interaction can be used to calculate the energy of
 - The whole
 - The parts
 - The interaction between the parts

This will be particularly useful when we discuss scission later on!

Constrained Hartree Fock

Example:



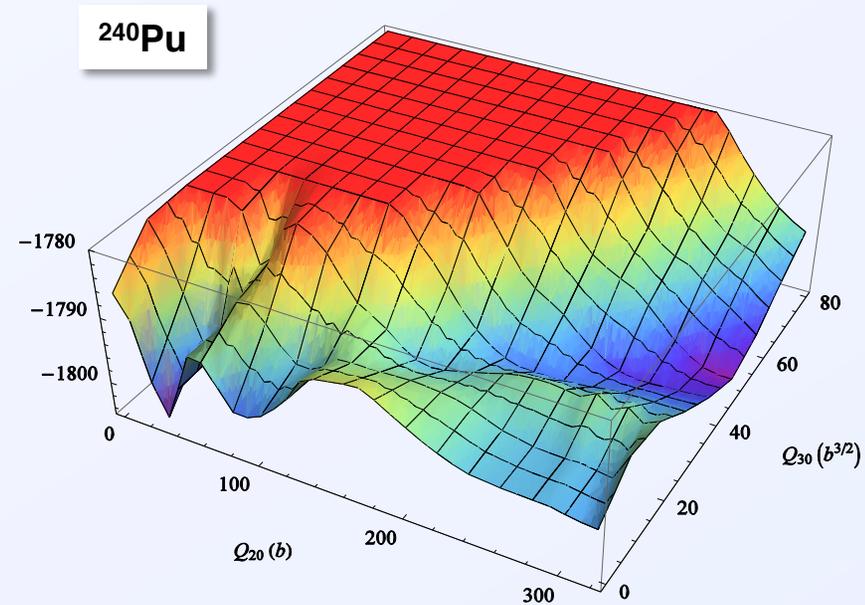
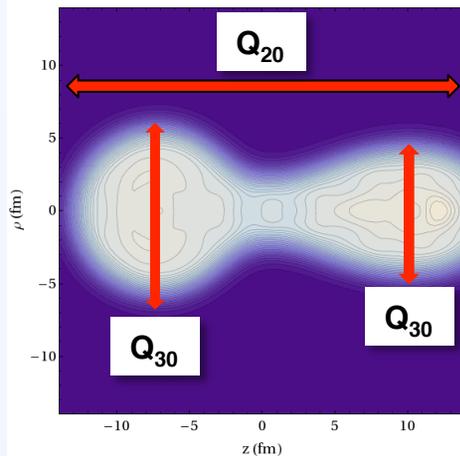
- Two minima in potential
- How do we reach both minima with Hartree Fock?
- Add a constraint to the minimization process via the method of Lagrange multipliers:

$$\delta \langle \text{HF} | \hat{H} - \lambda \hat{Q} | \text{HF} \rangle = 0$$

In fact, with constraints we can explore the entire potential energy curve (and not just the minima)

Example of constraints: quadrupole and octupole moments

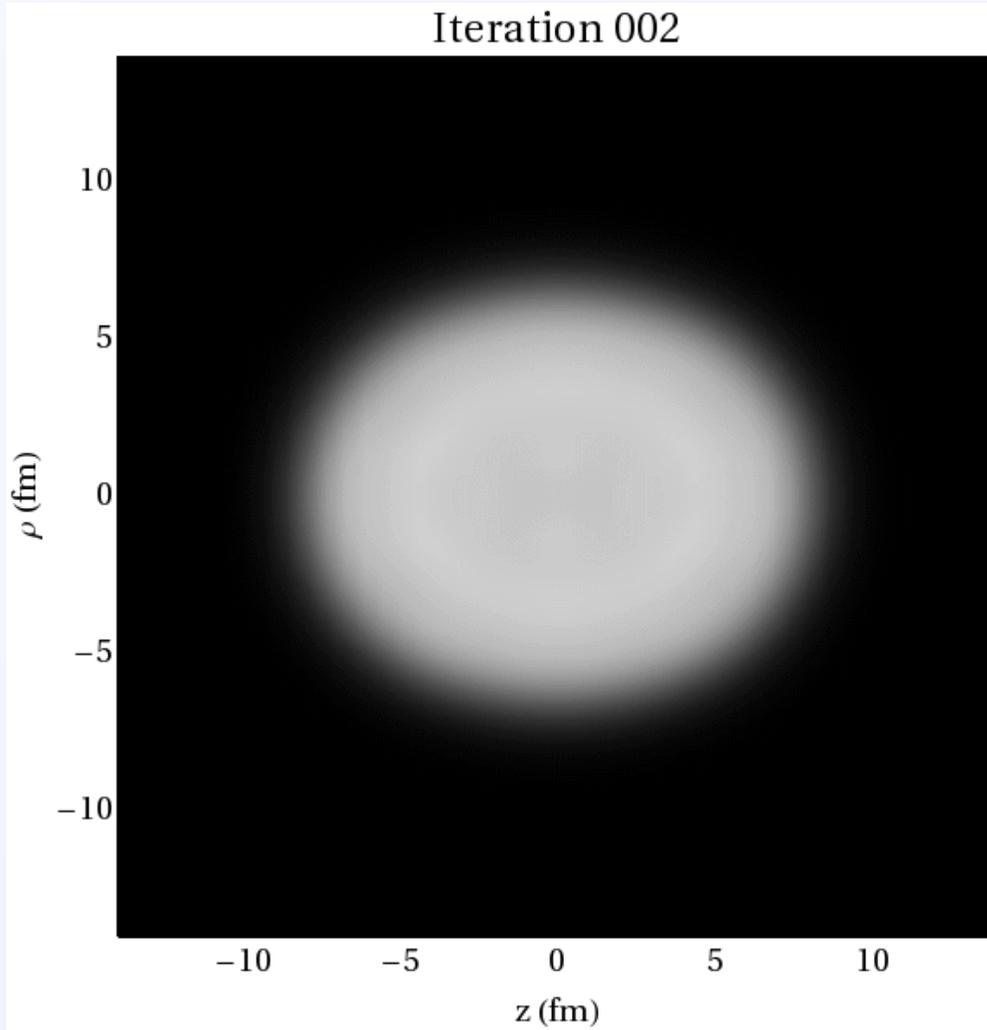
$|\Phi(q)\rangle = \text{mean-field solution at } q = \{Q_{20}, Q_{30}\}$



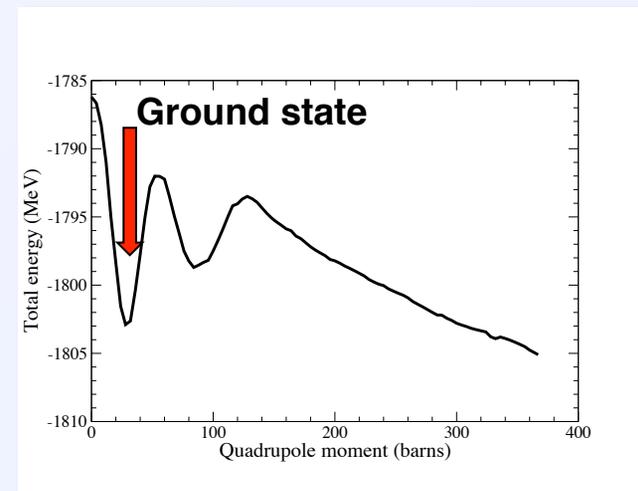
$$\langle \hat{Q}_{\ell m} \rangle = \int Y_{\ell m}^*(\theta, \phi) r^\ell \rho(\vec{x}) d^3x$$

Q_{20} controls “stretching” of nucleus
 Q_{30} controls mass asymmetry

Example: ground state of ^{240}Pu

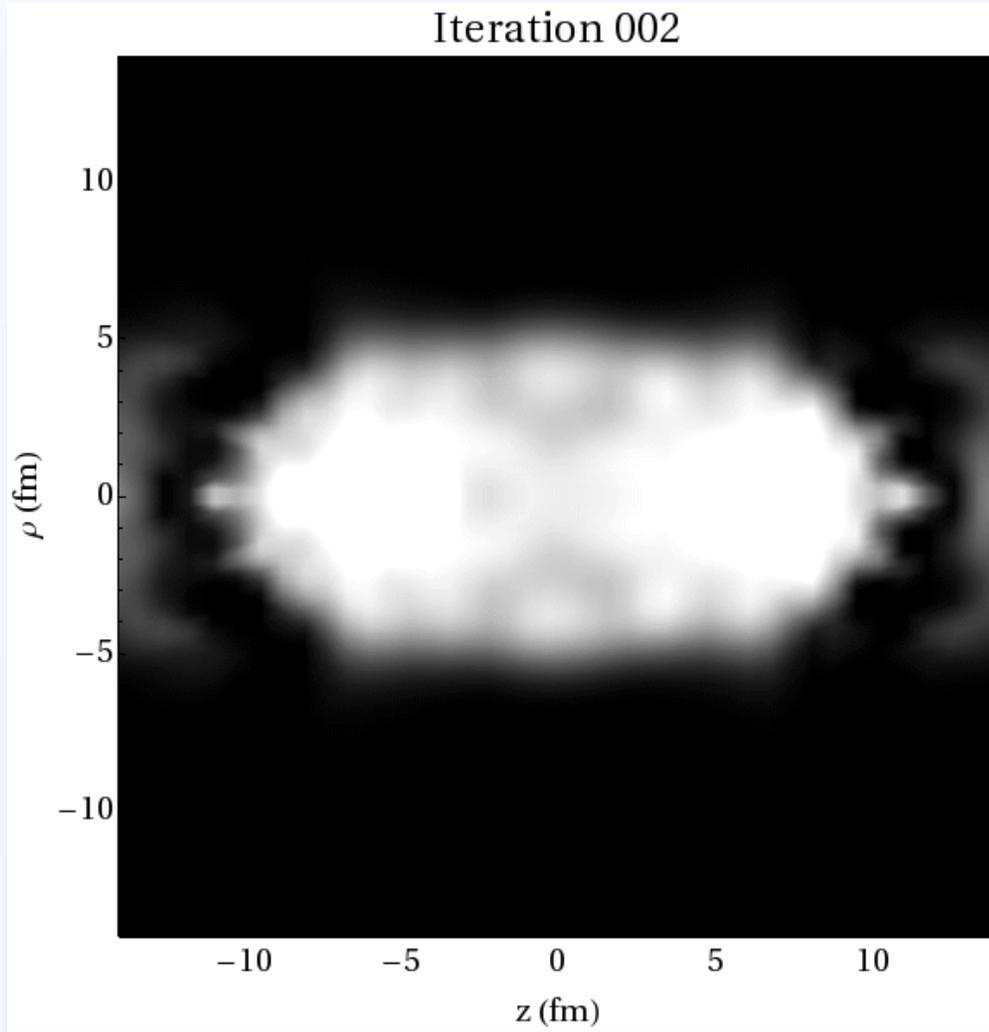


- Initial state = Slater determinant on deformed harmonic oscillator basis

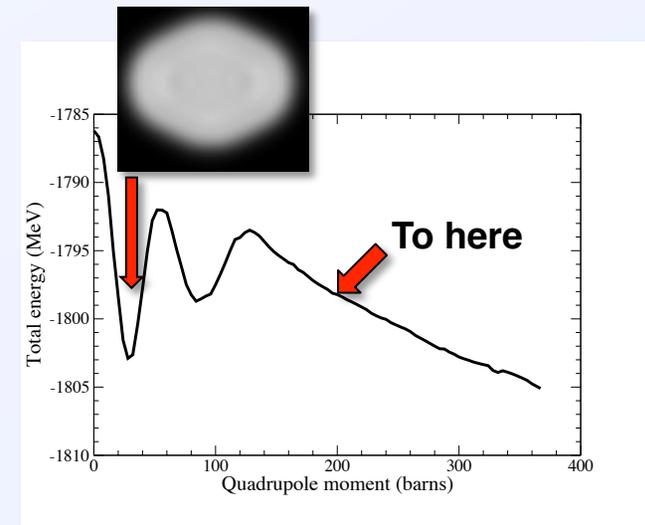


- Density settles rapidly into ground-state configuration (variational methods love minima!)

Example: deformed state of ^{240}Pu with $Q_{20} = 200 \text{ b}$

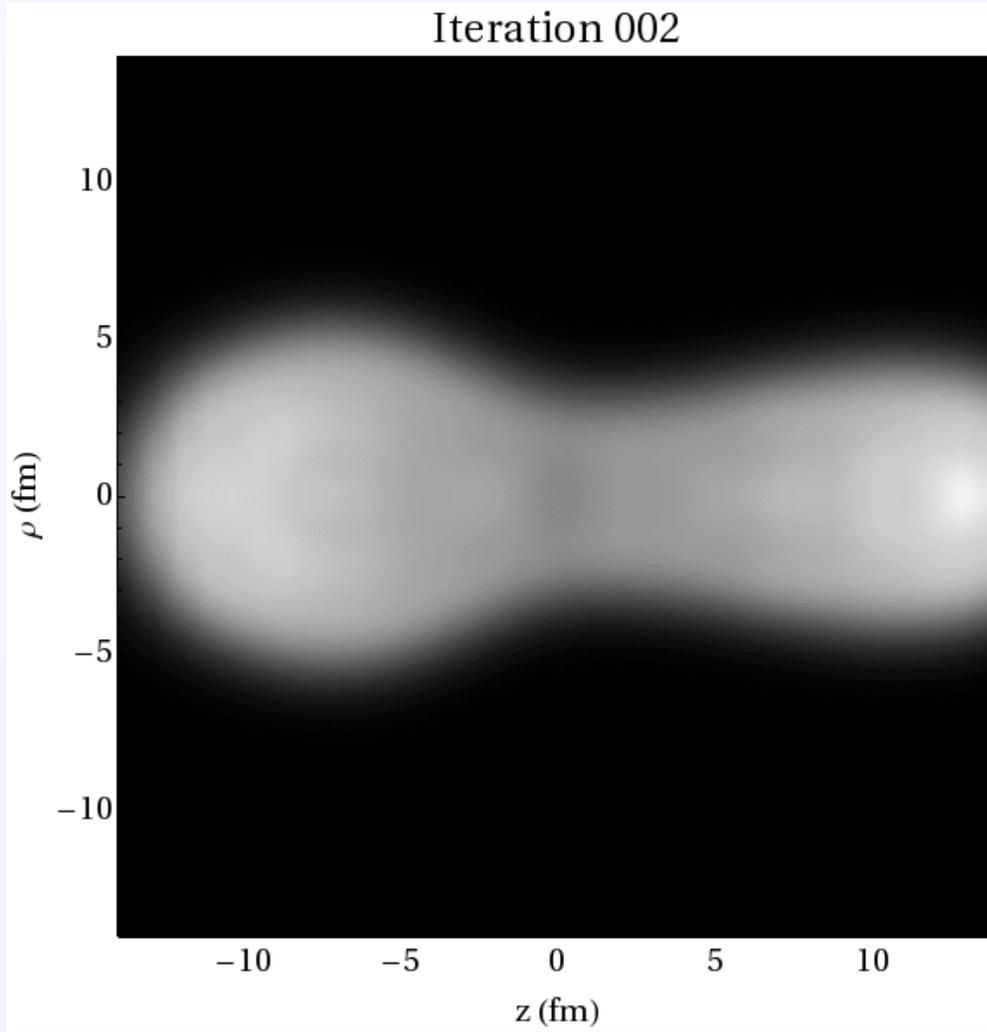


- Starting point is ground state solution:

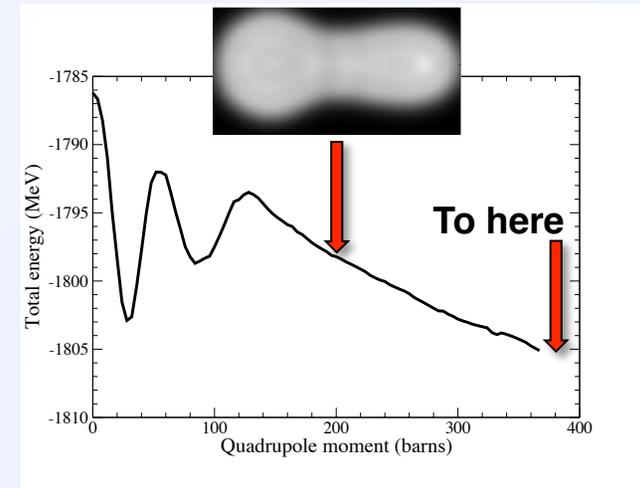


- Need constraint on Q_{20}
- Converges much more slowly
- Note mass asymmetry

Example: deformed state of ^{240}Pu with $Q_{20} = 380$ b



- Starting point is $Q_{20} = 200$ b solution:



- Need constraint on Q_{20}
- Converges very slowly
- Note that we have reached scission!

Excitation mechanisms of the nucleus

Not a nucleus, but will do for now



Simplest: particle-hole excitation



More complex configurations can be built from a multitude of simpler particle-hole excitations

Collective motion in a “classical” movie:



then



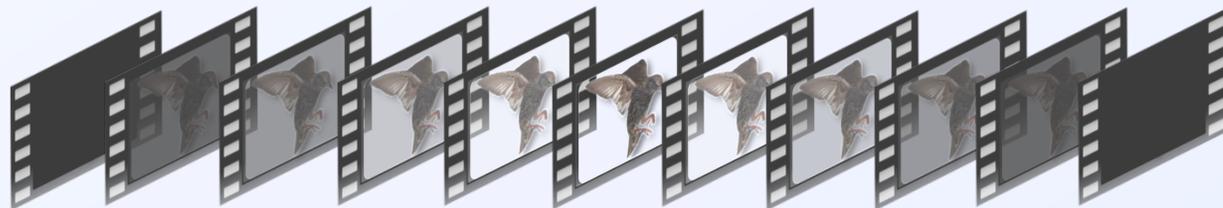
then



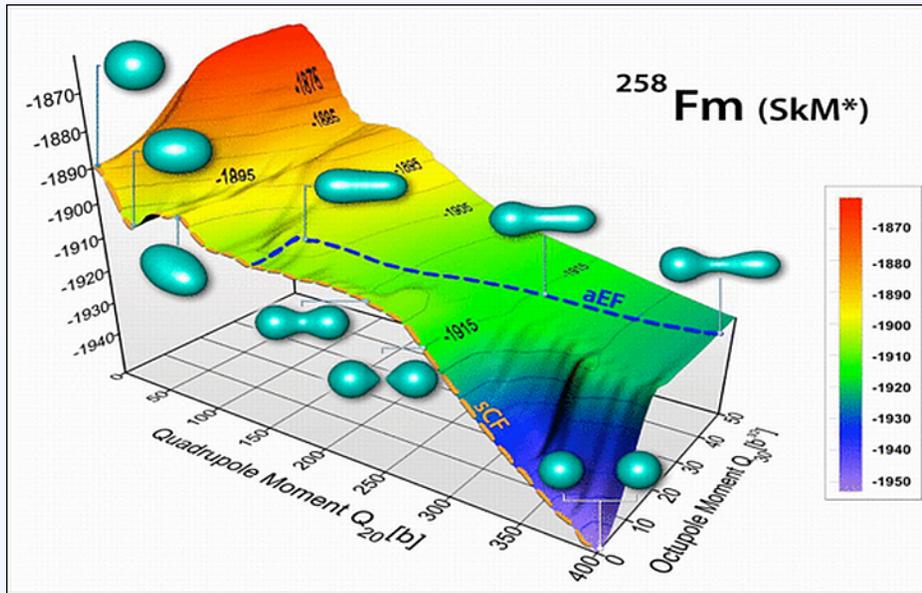
then...

The “quantum” movie of large-amplitude collective motion

- All frames for all possible flight paths and all possible configurations exist at the same time
- The “brightness” of each frame is what changes as a function of time
- All these frames, each with its own brightness, are shown at the same time



Building collective motion from single particles: the nucleus



From ascr-discovery.science.doe.gov
Credit: A. Staszczak et al., ORNL

- Each point on map is a single-particle configuration: HFB $\Rightarrow \Phi(q)$
- The nucleus explores many such configurations \Rightarrow form linear superposition of $\Phi(q)$:

$$|\Psi\rangle = \int dq f(q) |\Phi(q)\rangle$$

- Use variational procedure to determine the weights $f(q)$

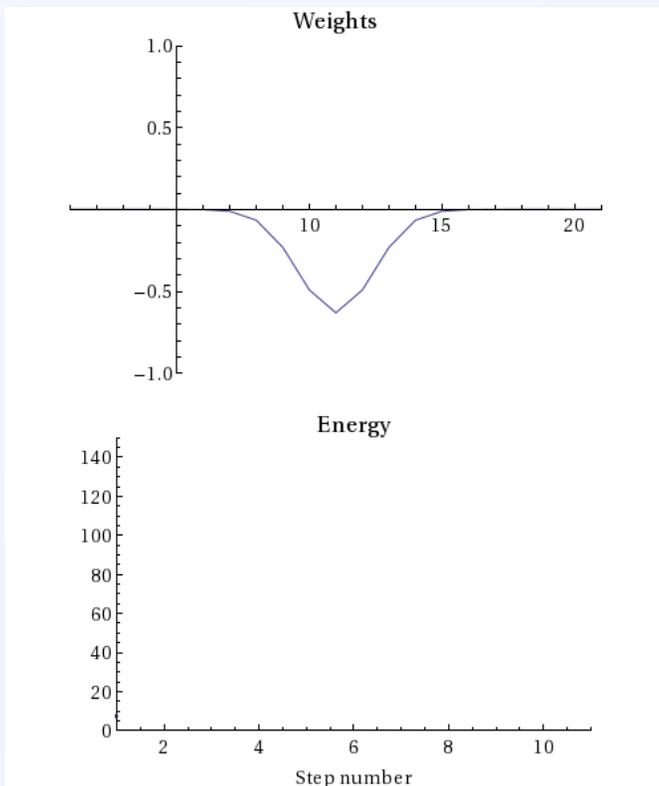
- This is the Generator Coordinate Method (GCM) first proposed by Hill & Wheeler in Phys. Rev. 89, 1106 (1953)
- A truly quantum-mechanical description of collectivity built from single-particle degrees of freedom

Calculations using the GCM

GCM wave function: $|\Psi\rangle = \int dq f(q)|\Phi(q)\rangle$

&

Variational principle: $\delta E = \delta \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0$



Numerical Example: harmonic oscillator

- Vary weights $f(q)$ smoothly
 - Look for stationary values in energy
- ⇒ **Spectrum of collective states**

For more complicated H, this is not practical

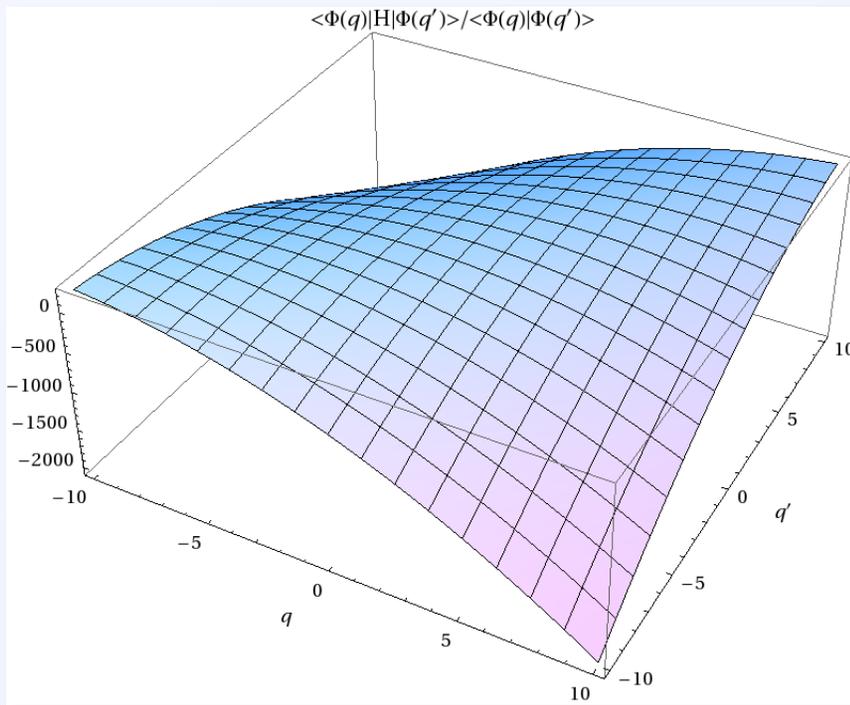
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Let's look at the Hamiltonian overlaps for the harmonic-oscillator example:



And switch to coordinates:

$$\bar{q} \equiv \frac{q + q'}{2}$$
$$\delta q \equiv q - q'$$

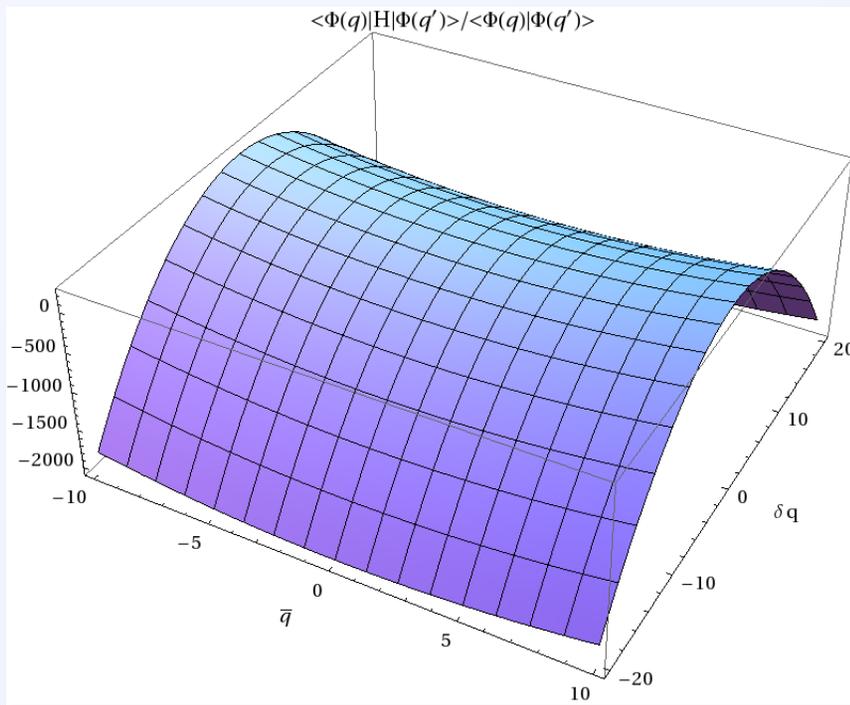
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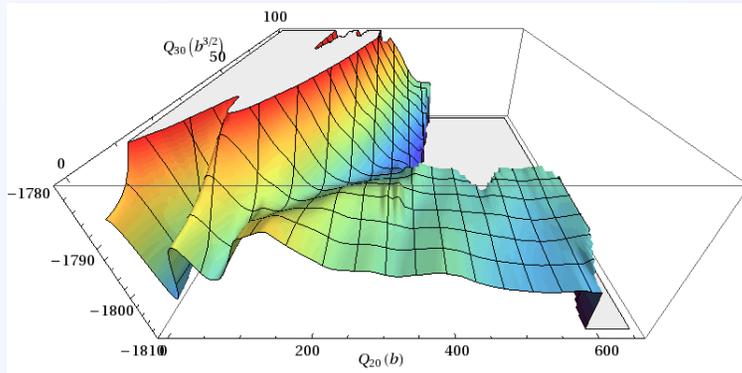
$$\delta q \equiv q - q'$$

Expand overlaps to 2nd order in δq

- For harmonic oscillator expansion is exact, otherwise it's an approximation
- ⇒ Schrodinger-like equation
- ⇒ Collective Hamiltonian
- In particular, curvature near $\delta q = 0$ is related to inertia of collective system

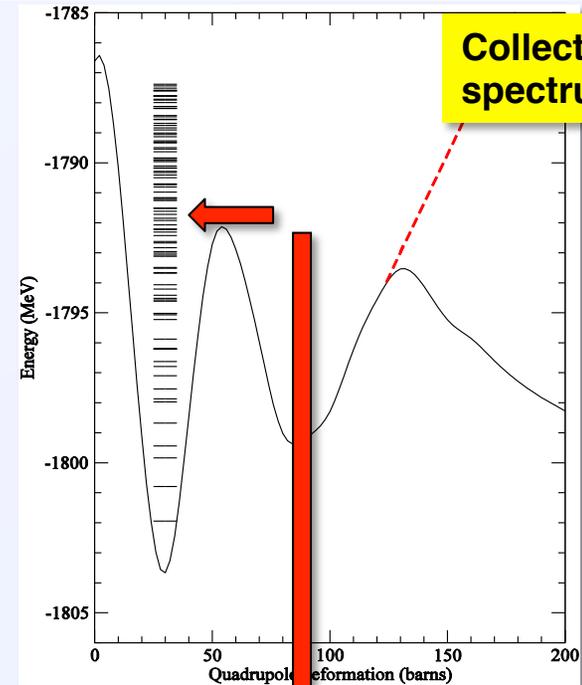
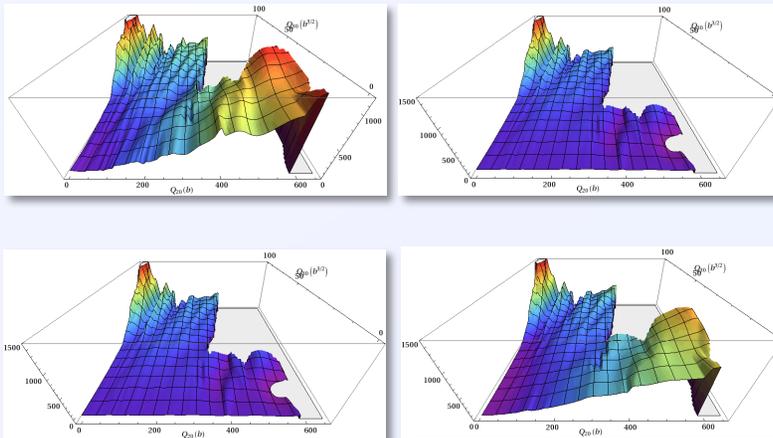
Application of the GCM: collective spectrum of ^{240}Pu in (Q_{20}, Q_{30})

Collective Hamiltonian:

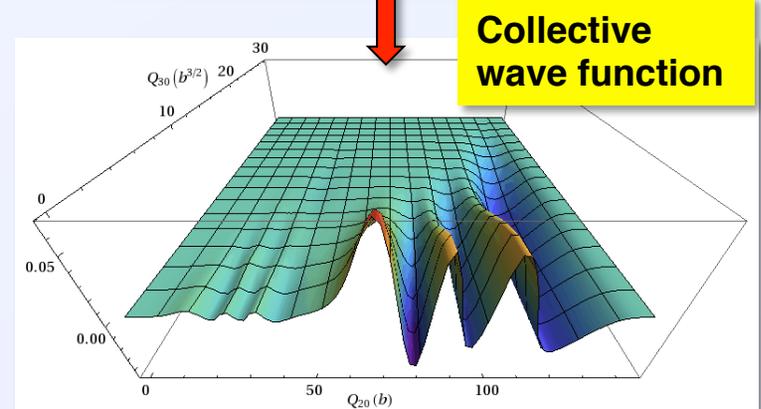


Potential surface:

Inertia tensor:



Collective spectrum



Collective wave function

Fission dynamics: the Time-Dependent Hartree-Fock method

- In general: $|\Psi(t)\rangle = \exp(-iHt/\hbar) |\Psi(0)\rangle$
 - For $H =$ full many-body Hamiltonian, this is too difficult!
- Time-dependent Hartree-Fock (Bogoliubov)
 - Start with Slater determinant, assume it stays a Slater determinant
 - From variational principle:
$$\delta \int_{t_1}^{t_2} dt \left\langle \Psi \left| \hbar i \frac{\partial}{\partial t} - H \right| \Psi \right\rangle = 0$$
 With Ψ a Slater determinant
 - The good:
 - introduces internal excitations through particle collisions
 - no need to choose collective coordinates a priori, the system finds its path on the energy surface
 - The bad:
 - Classical behavior (system follows a single trajectory)
 - Can't tunnel (due to conservation of energy)
 - Spurious final state interaction



Some developments in TDHF as a tool for fission

- J.W. Negele et al., Phys. Rev. 17, 1098 (1978)
 - Calculated ^{236}U induced fission times, compared with different dissipations/viscosities. Found fission times of $3\text{-}4 \times 10^{-21}$ s
- K. Dietrich and J. Nemeth, Z. Phys. A 300, 183 (1981)
 - Studied fission of slabs of nuclear matter
- J. Okolowicz, et al., J. Phys. G 9, 1385 (1983)
 - Compared calculations with one- or two-center Slater determinants
- A. S. Umar et al., J. Phys. G 37, 064037 (2010)
 - TDHF with constrained density, applied to the study of fission following heavy-ion collisions (e.g., $^{100}\text{Zr} + ^{140}\text{Xe}$)
- D. Lacroix, Phys. Rev. C 73, 044311 (2006): Stochastic TDHF: quantum jumps between Slater determinants
- I Stetcu et al., Phys. Rev. C 84, 051309 (2011): time-dependent density-functional theory

Could TDHF provide insight into the relevant degrees of freedom throughout the fission process?



Fission dynamics: the time-dependent GCM

Replace the GCM ansatz with: $|\Psi(t)\rangle = \int dq f(q,t) |\Phi(q)\rangle$



Variational principle + 2nd order expansion in non-locality

$$\delta \int_{t_1}^{t_2} dt \left\langle \Psi \left| \hbar i \frac{\partial}{\partial t} - H \right| \Psi \right\rangle = 0$$

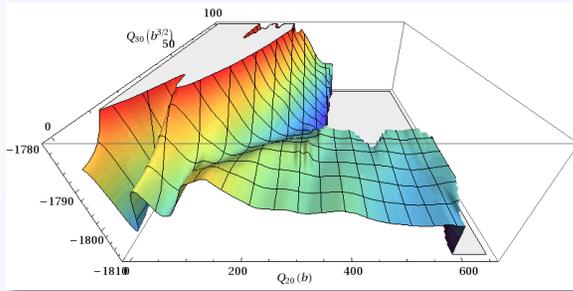
With Ψ a superposition of Slater determinants (or HFB states)

- To obtain microscopic, time-dependent picture of fission:
 - Calculate potential energy surface, inertia tensor, and initial state
 - Solve time-dependent collective Schrodinger equation
- See: J.-F. Berger et al., *Comp. Phys. Comm.* 63, 365 (1991); H. Goutte et al., *Phys. Rev. C* 71, 024316 (2005)

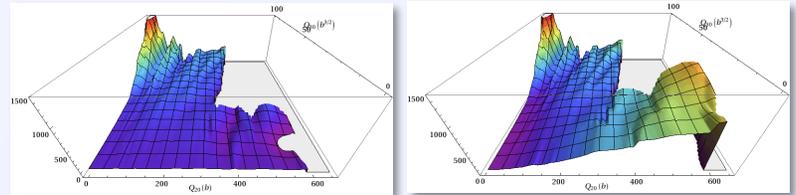
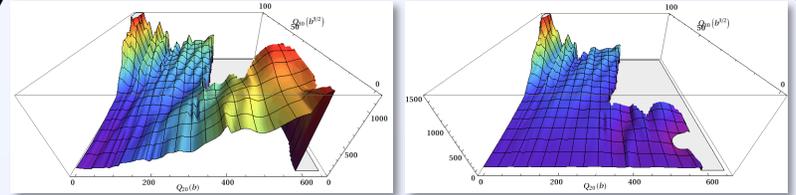


Application of the GCM: fission dynamics for ^{240}Pu

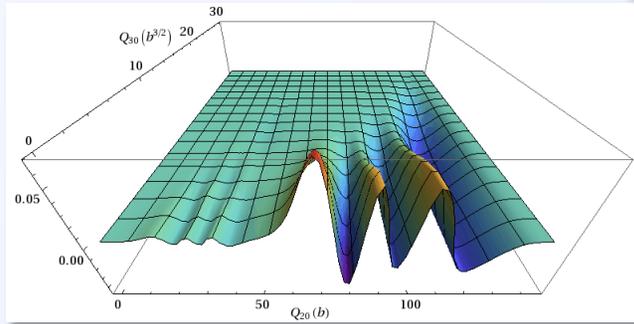
Potential surface:



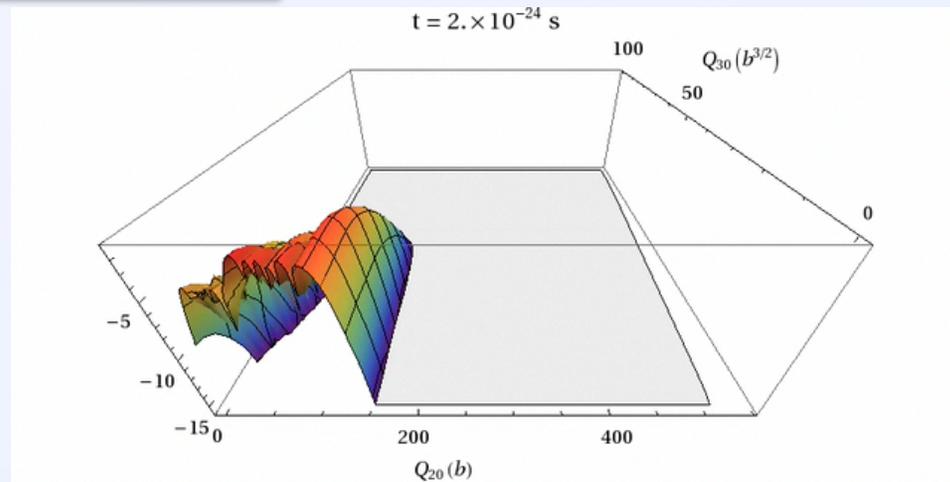
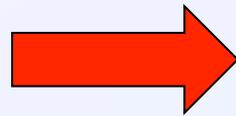
Inertia tensor:



Initial state



$$\log |g(t)|^2$$



Coupling between intrinsic and collective excitations in fission

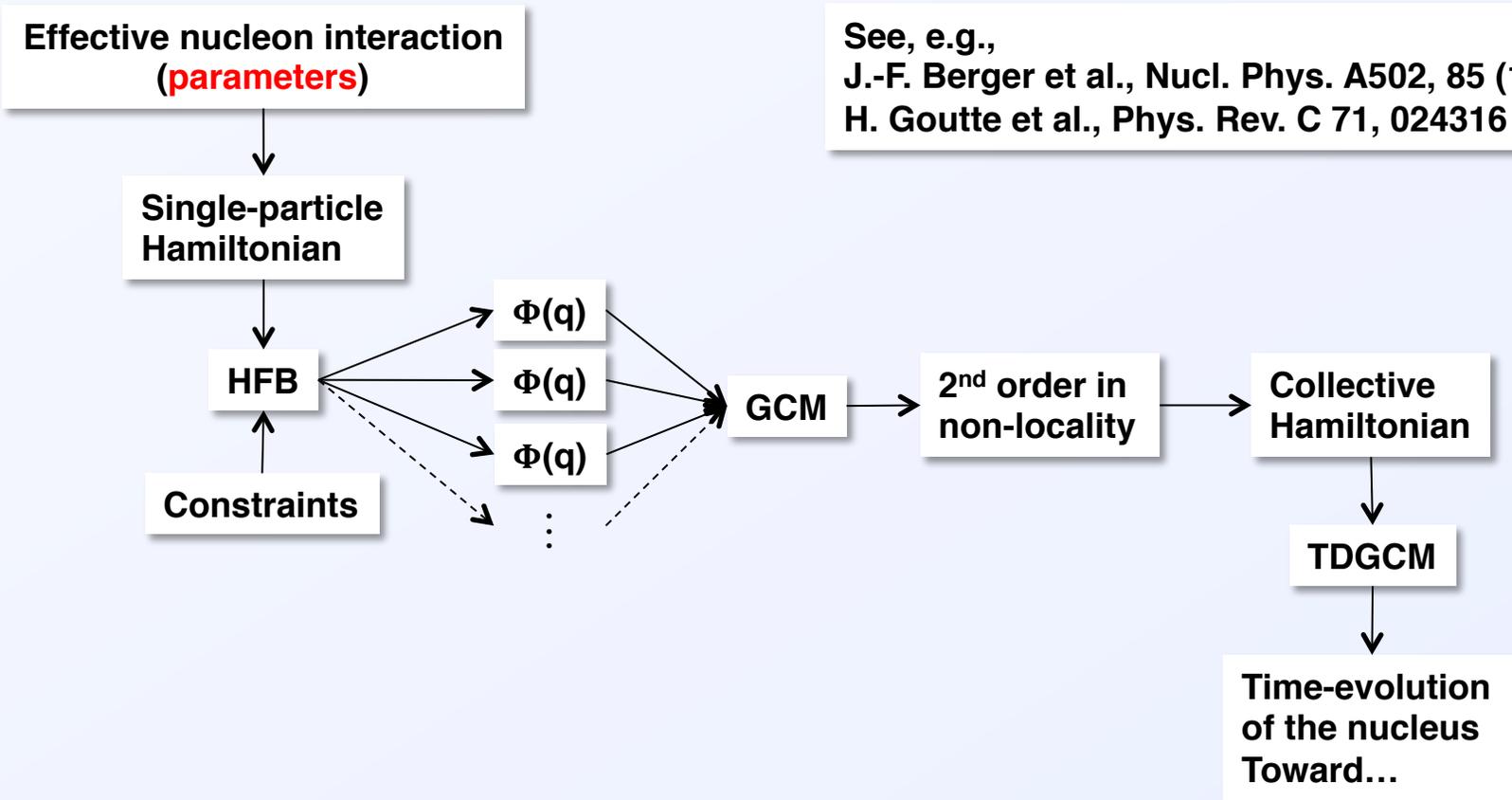
- Develop GCM on a basis that includes intrinsic excitations

$$|\Psi\rangle = \int dq f_0(q) \underbrace{|\Phi_0(q)\rangle}_{\text{HFB minima}} + \sum_{i \neq 0} \int dq f_i(q) \underbrace{|\Phi_i(q)\rangle}_{\text{excitations}}$$

- Leads to generalized, non-adiabatic, Hill-Wheeler equation
- Can be reduced to Schrodinger-like equation
 - Coupling between HFB minima and excited states is treated explicitly
- This promising approach is in development
 - See Bernard et al., Phys. Rev. C 84, 044308 (2011)



Recap: the microscopic approach so far



See, e.g.,
J.-F. Berger et al., Nucl. Phys. A502, 85 (1989)
H. Goutte et al., Phys. Rev. C 71, 024316 (2005)

We're missing a crucial ingredient: scission



A Microscopic Theory of Fission (part II)

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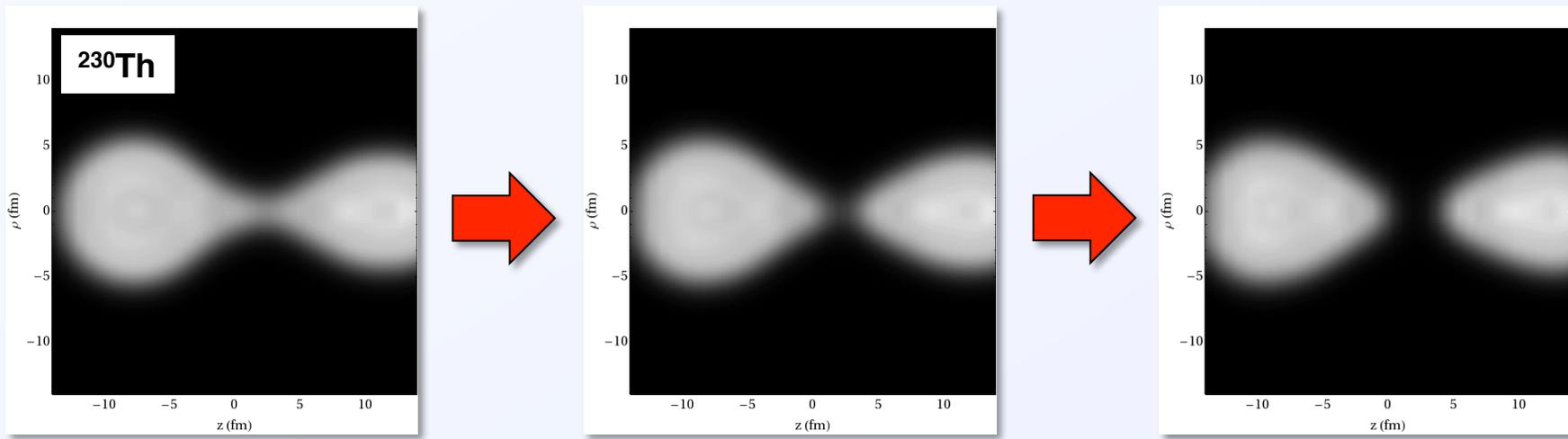
W. Younes

Physical and
Life Sciences

Lawrence Livermore National Laboratory

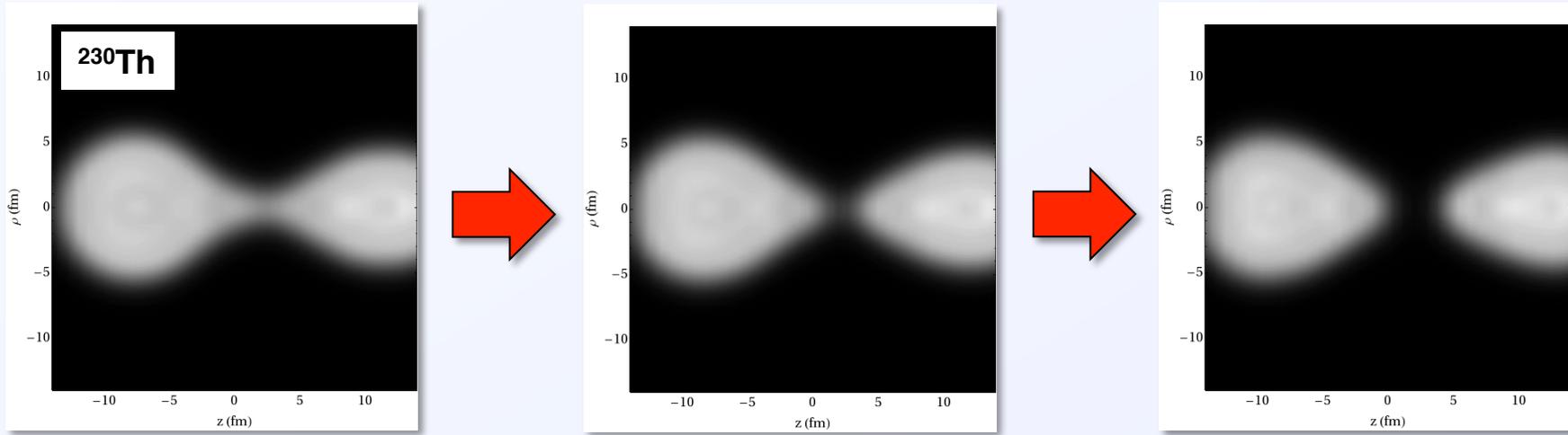
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Security, LLC, Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

The nucleus near scission



Microscopic calculation of the final stages of fission

The nucleus near scission

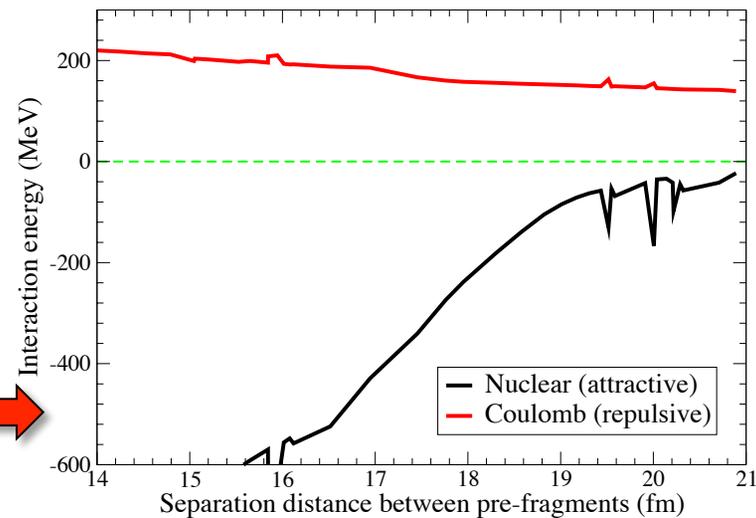


but calculate the nuclear interaction energy between fragments in last panel:

$$E_{\text{int}} = -68.3 \text{ MeV}$$

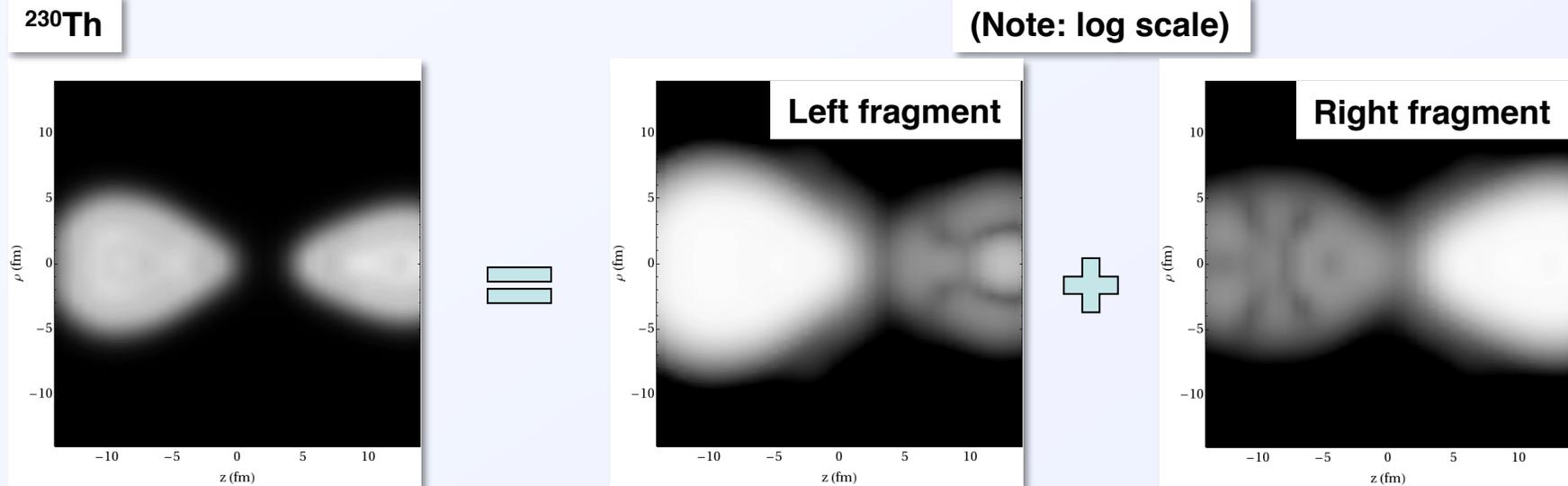
Not negligible!

In fact, look as a function of fragment separation:



So where does scission occur?

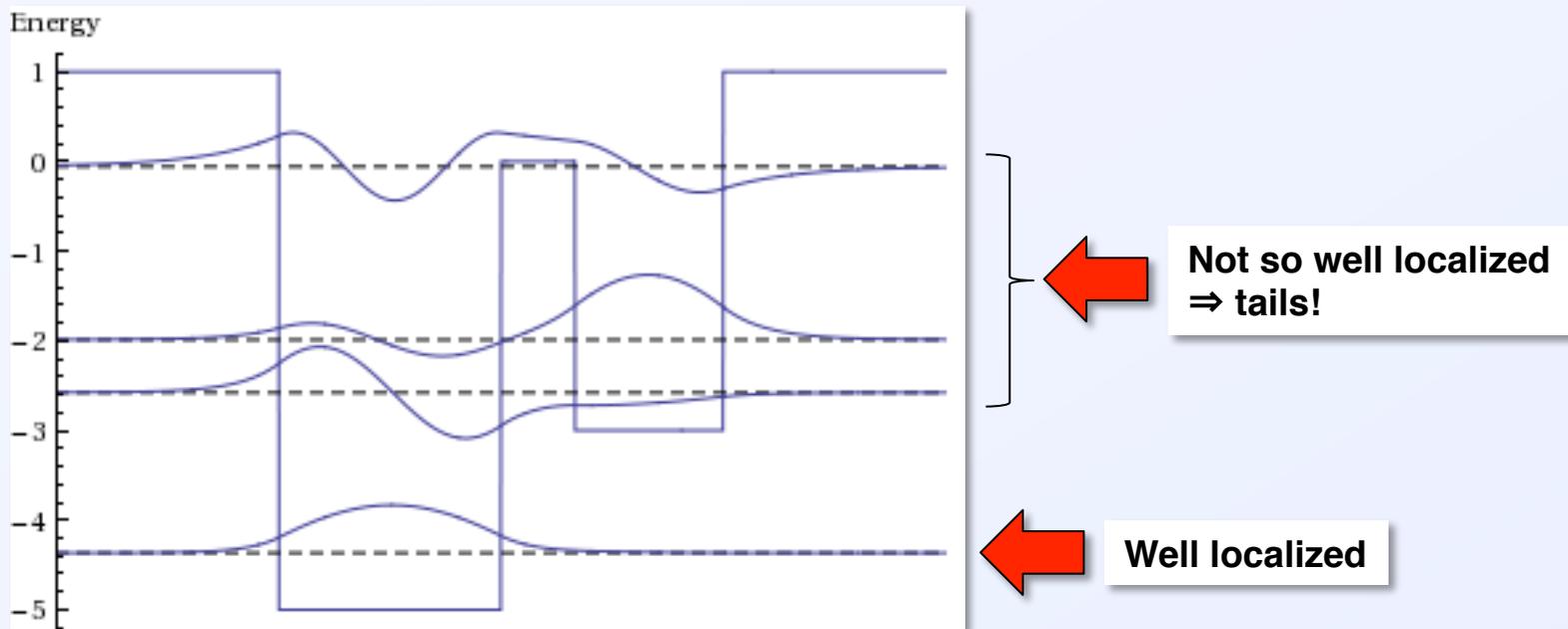
The nucleus near scission



- The nucleon wave functions are delocalized, i.e., the fragments have tails!
- Tails are small but venture deep into complementary fragment!
 - Keep in mind: total nuclear energy of ^{230}Th in G.S. ~ -6.6 GeV
 - Each particle in tails contributes ~ -50 MeV to nuclear interaction between fragments
- We are dealing here with the non-local nature of quantum mechanics!

The quantum localization problem in a simple model

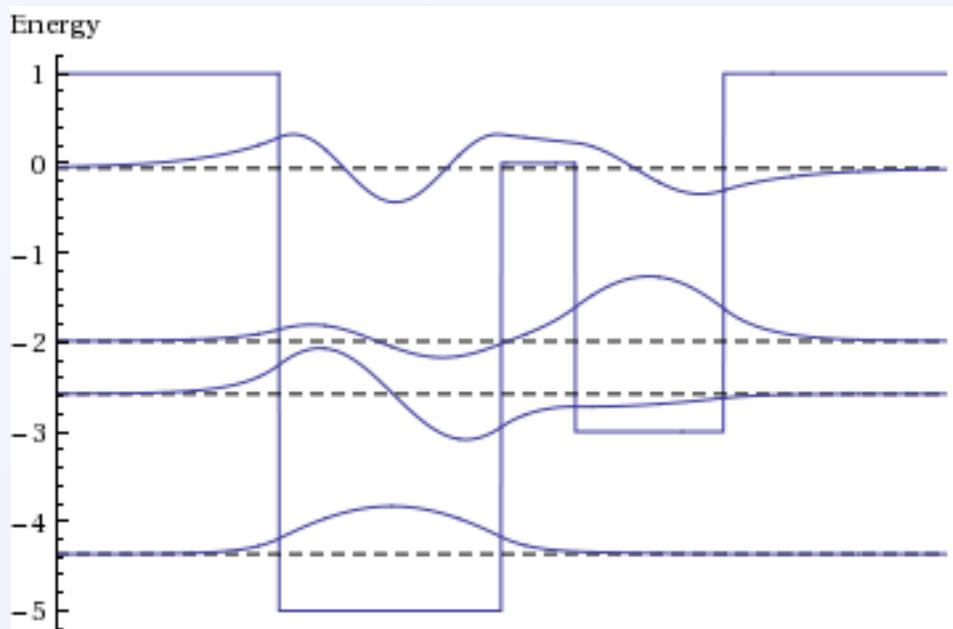
- In QM, the double-well potential gives rise to delocalized orbitals (see, e.g., R. Gilmore, “Elementary Quantum Mechanics in One Dimension”, JHU press (2004))



This is not a numerical issue, a basis problem, or a problem that is unique to nuclear fission: it is a direct consequence of the non-local nature of QM

The quantum localization problem in a simple model

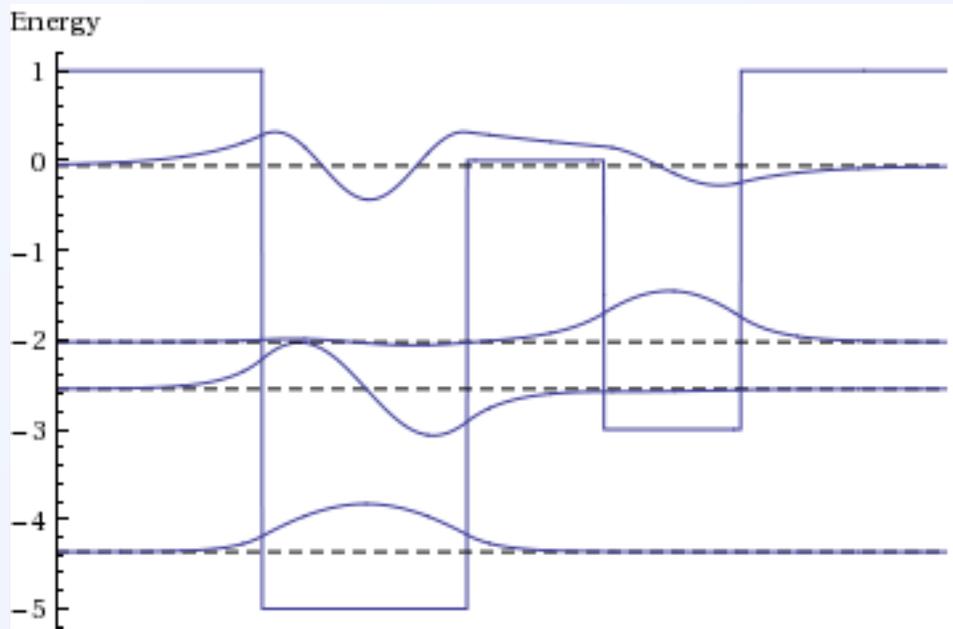
- In QM, the double-well potential gives rise to delocalized orbitals (see, e.g., R. Gilmore, “Elementary Quantum Mechanics in One Dimension”, JHU press (2004))



Moving the wells apart does seem to reduce the tails: problem solved?

The quantum localization problem in a simple model

- In QM, the double-well potential gives rise to delocalized orbitals (see, e.g., R. Gilmore, “Elementary Quantum Mechanics in One Dimension”, JHU press (2004))



**When accidental degeneracies occur, the tails come back!
This is what happens in the fission problem**

The concept of Localized Molecular Orbitals (LMOs)

Sir John Lennard-Jones, Proc. Roy. Soc. A 198, 14 (1949):

The equations (2.01) were obtained from a determinantal wave function of the form

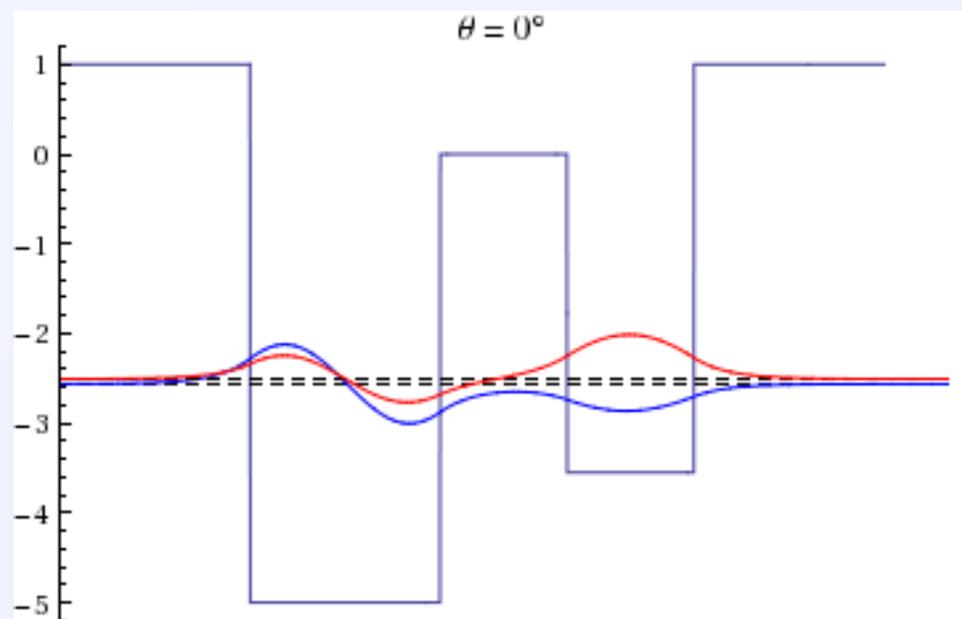
$$\Phi = \text{Det}\{\psi_1(1)\alpha(1)\psi_1(2)\beta(2)\dots\psi_p(2p-1)\alpha(2p-1)\psi_p(2p)\beta(2p) \\ \times \psi_{p+1}(2p+1)\alpha(2p+1)\dots\psi_{p+q}(2p+q)\alpha(2p+q)\}, \quad (3.01)$$

and the properties of the system will not be altered by any transformation which leaves this wave function unchanged. Thus any orthonorm transformation of the functions ψ_1 to ψ_n , which constitute its elements, will not change Φ . It is unchanged

Let's go back to our simple example and mix the two degenerate states with a rotation through angle θ



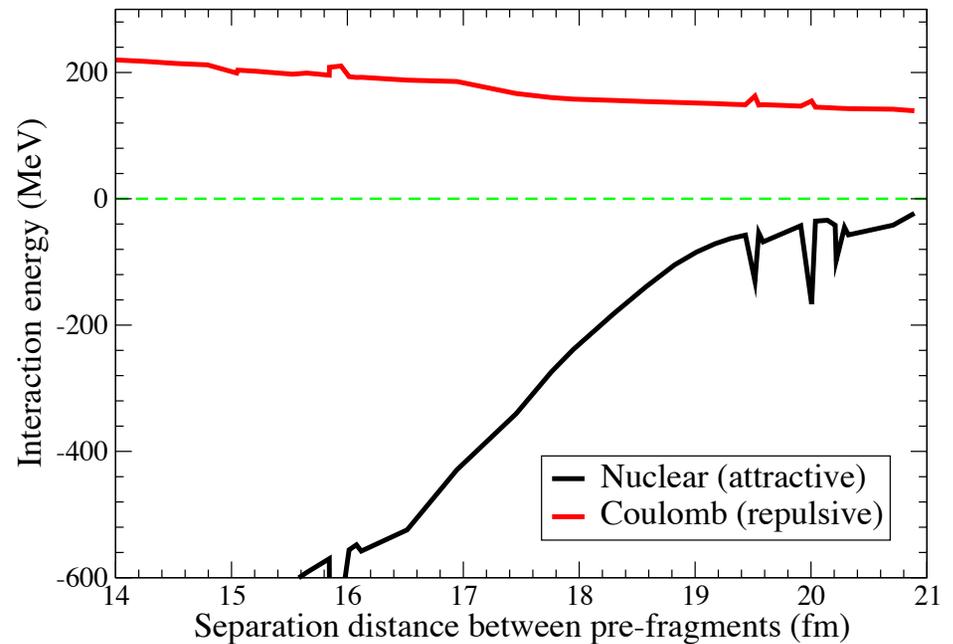
This is in the spirit of the “Localized Molecular Orbitals” used in molecular physics to construct physically meaningful orbitals (e.g., core, valence, bond) from delocalized Hartree-Fock solutions.



For fission: choose representation (i.e. transformation) that is appropriate to scission!

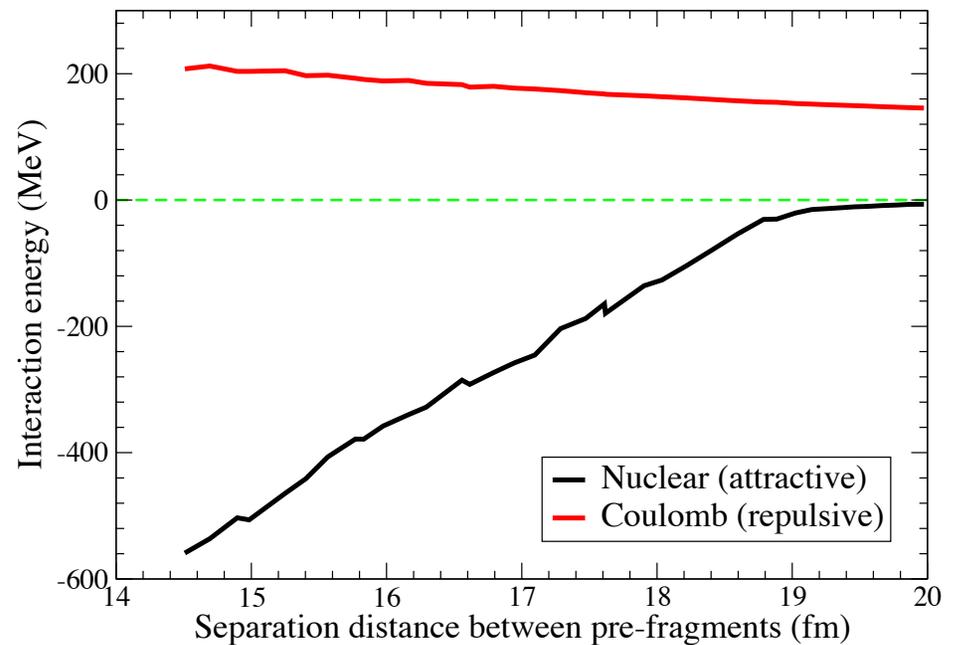
The nucleus near scission: quantum localization

- Remember: before quantum localization



The nucleus near scission: quantum localization

- Now: find a unitary transformation that reduces the tails
- ⇒ we can describe fission up to scission, and beyond



Younes & Gogny, Phys. Rev. Lett. 107, 132501 (2011)

We have a quantum-mechanical definition of scission!

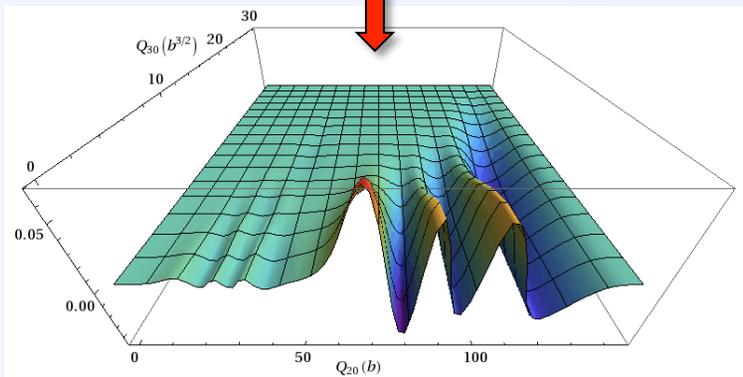
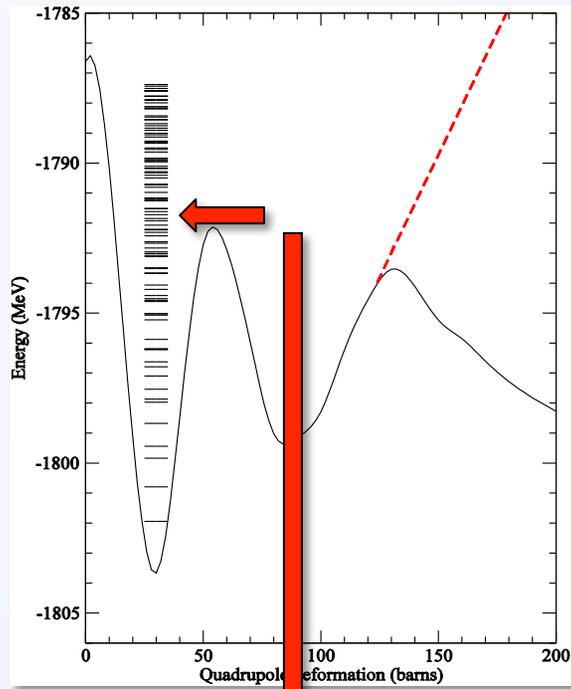
The quantum-mechanical definition of scission

- 1) Coulomb force \gg nuclear attraction between pre-frags (e.g., $\times 30$)
- 2) Exchange interaction is small (e.g., < 1 MeV)
 - \Rightarrow To good approx, can neglect antisymmetry between fragments
 - $\Rightarrow |\tilde{0}\rangle \approx |\tilde{0}\rangle_1 \times |\tilde{0}\rangle_2$ for all quantities of interest (energies, moments,...)
- 3) Can excite local set of 2-qp states on each fragment

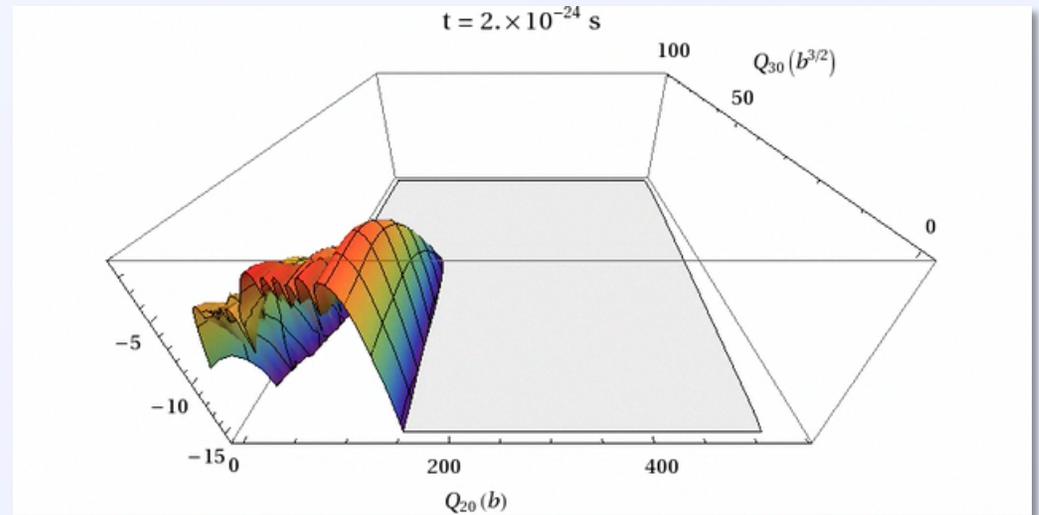
Fragments are separate entities, with their own excitations, and interacting only through a repulsive force acting only on their respective centers of mass



Calculating fission yields



Recall the discussion of the TDGCM

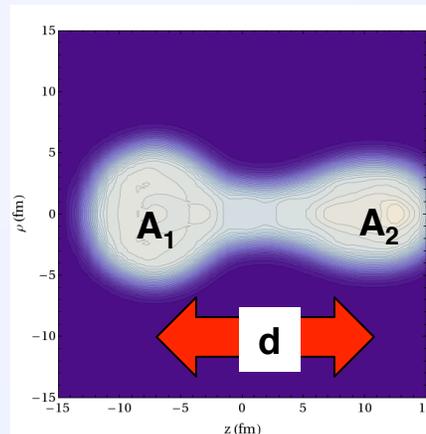


We have a wave packet evolving toward the scission configurations

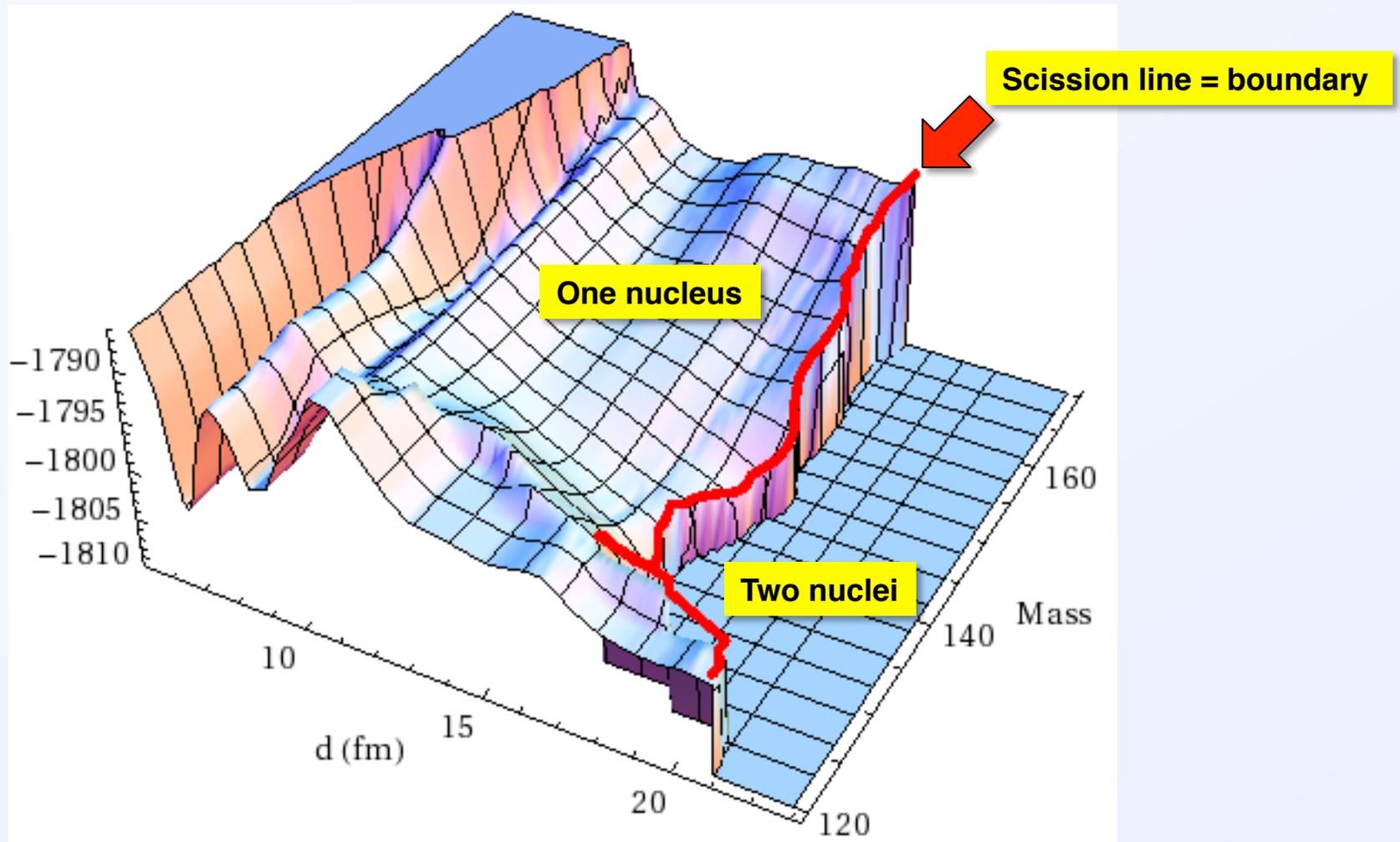
We need better collective coordinates near scission

- We want scission point for each mass division
- Traditionally: Q_{30} used to explore different mass divisions
- In practice: there isn't a one-to-one relation between Q_{30} and A
- As the nucleus nears scission, local constraints (constraints on the individual pre-fragments) become important
- So, instead of Q_{20} and Q_{30} , we work with:

$$d \equiv z_2 - z_1$$
$$\xi \equiv \frac{A_2 - A_1}{A}$$

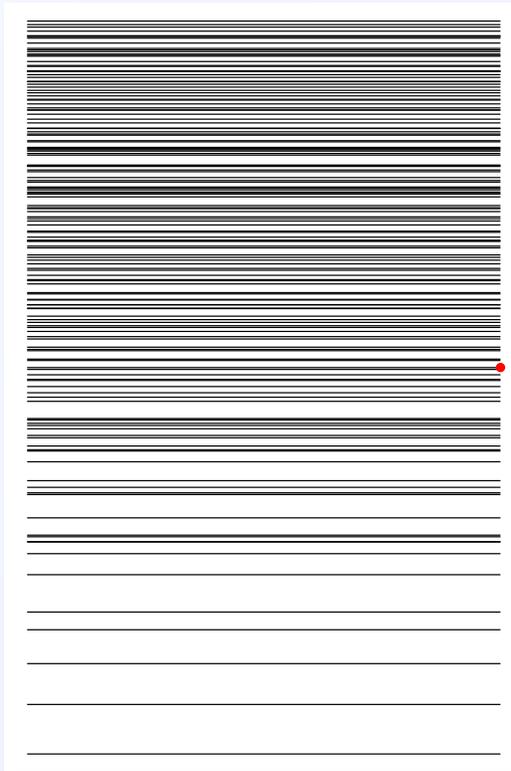


The scission line in the new coordinates

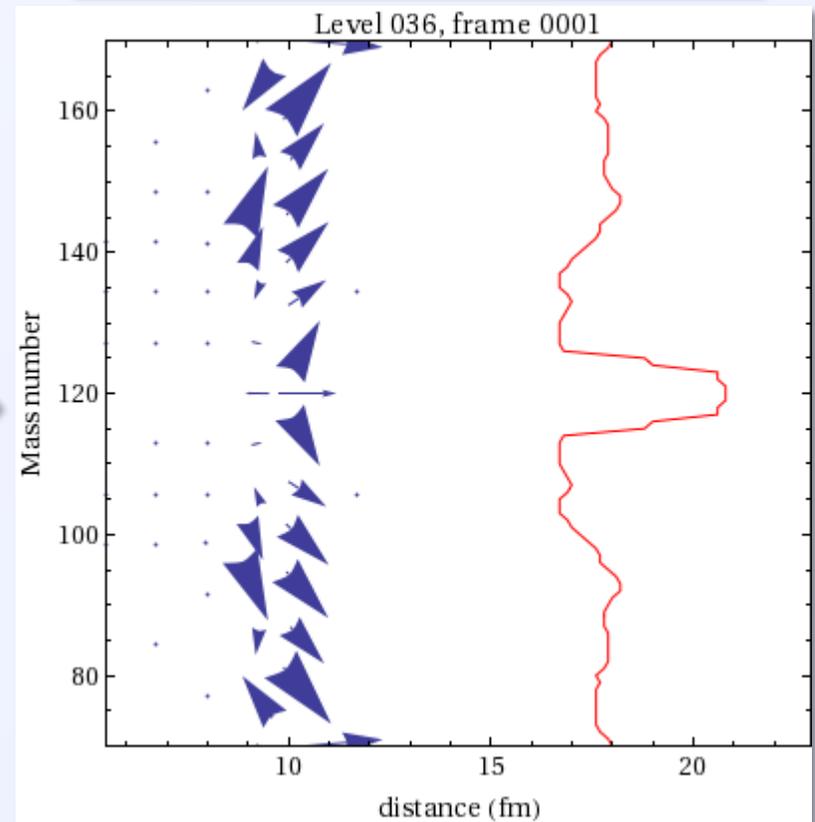


How do we get the probability of populating the scission points?

^{240}Pu collective levels from GCM

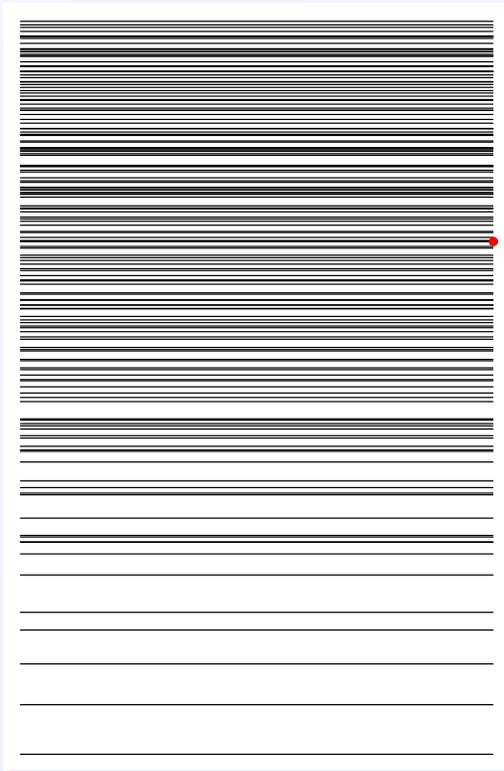


Time evolution of probability current

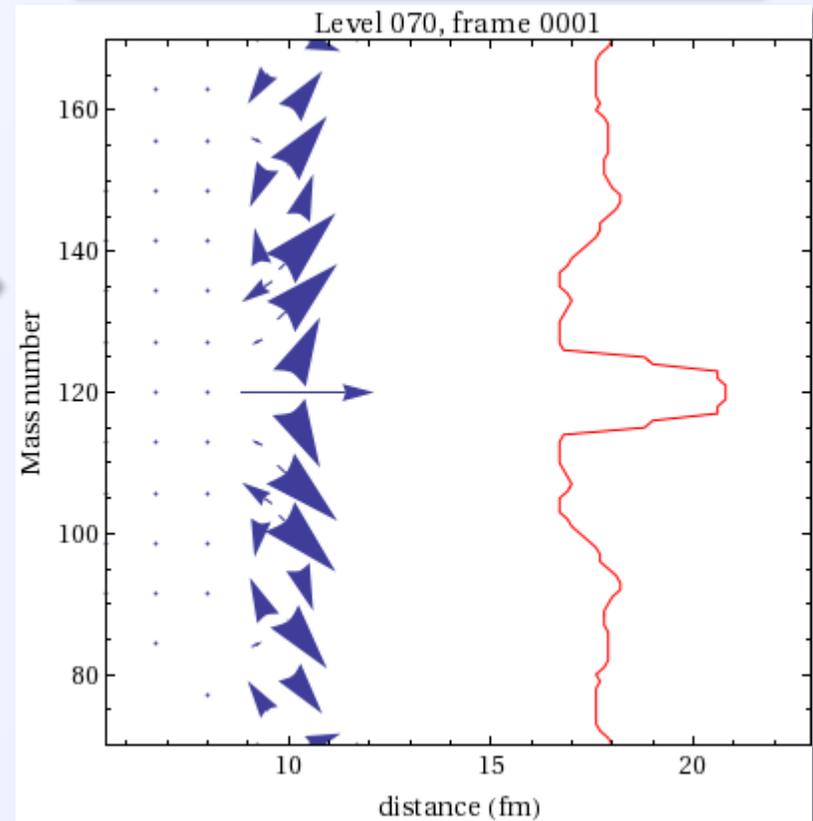


How do we get the probability of populating the scission points?

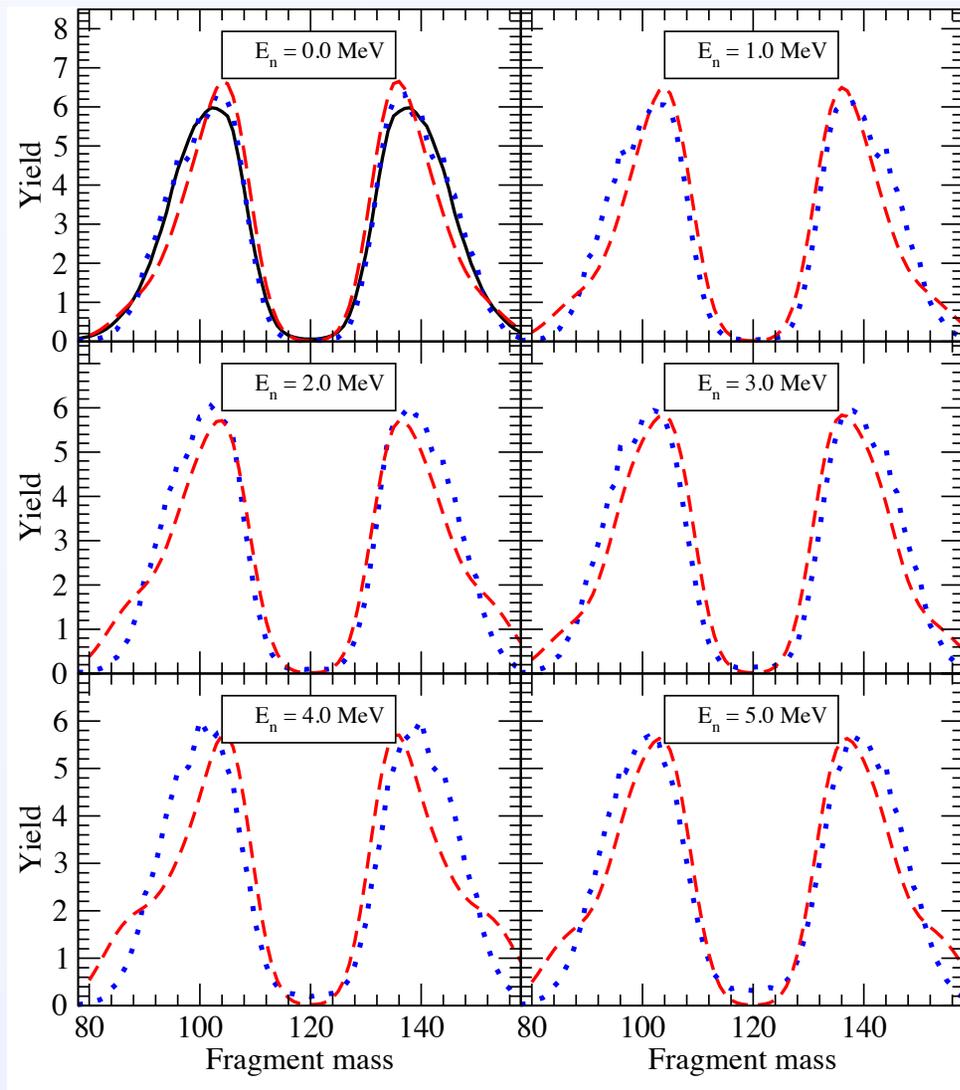
^{240}Pu collective levels from GCM



Time evolution of probability current



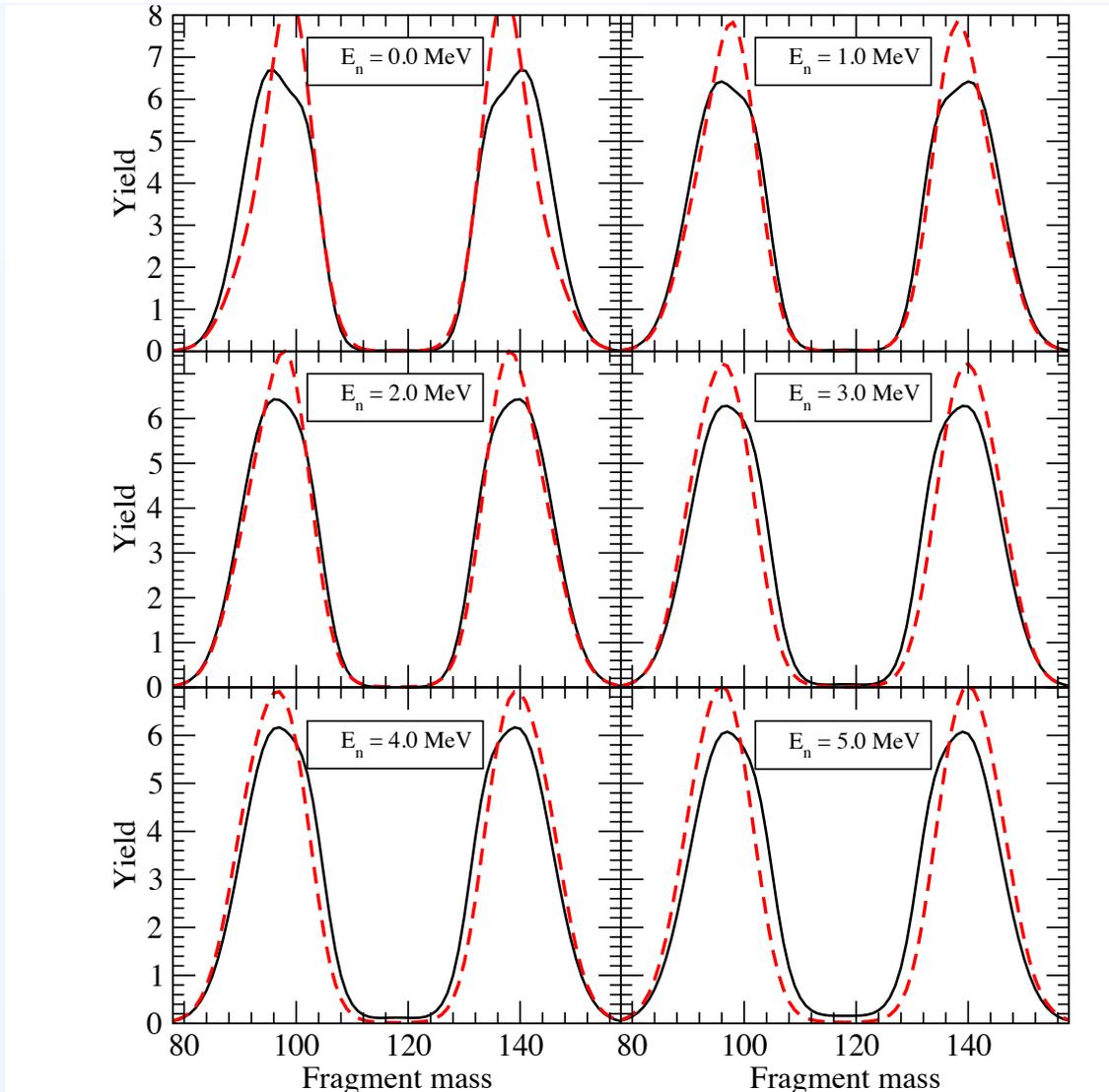
Fission dynamics: $^{239}\text{Pu}(n,f)$ mass distributions for $E_n = 0-5$ MeV



Younes et al., Proc. ICFN5, p. 605 (2012)



Fission dynamics: $^{235}\text{U}(n,f)$ mass distributions for $E_n = 0-5$ MeV

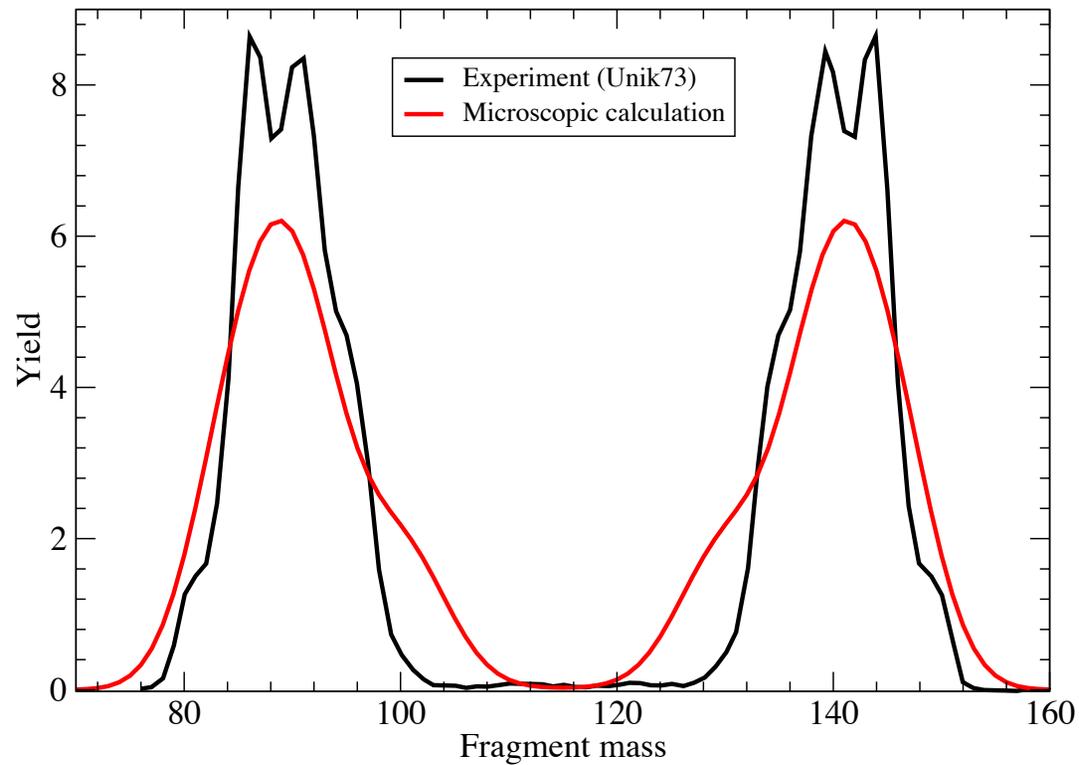


--- Microscopic calc
— Straede (87)

Younes et al., Proc. ICFN5, p. 605 (2012)

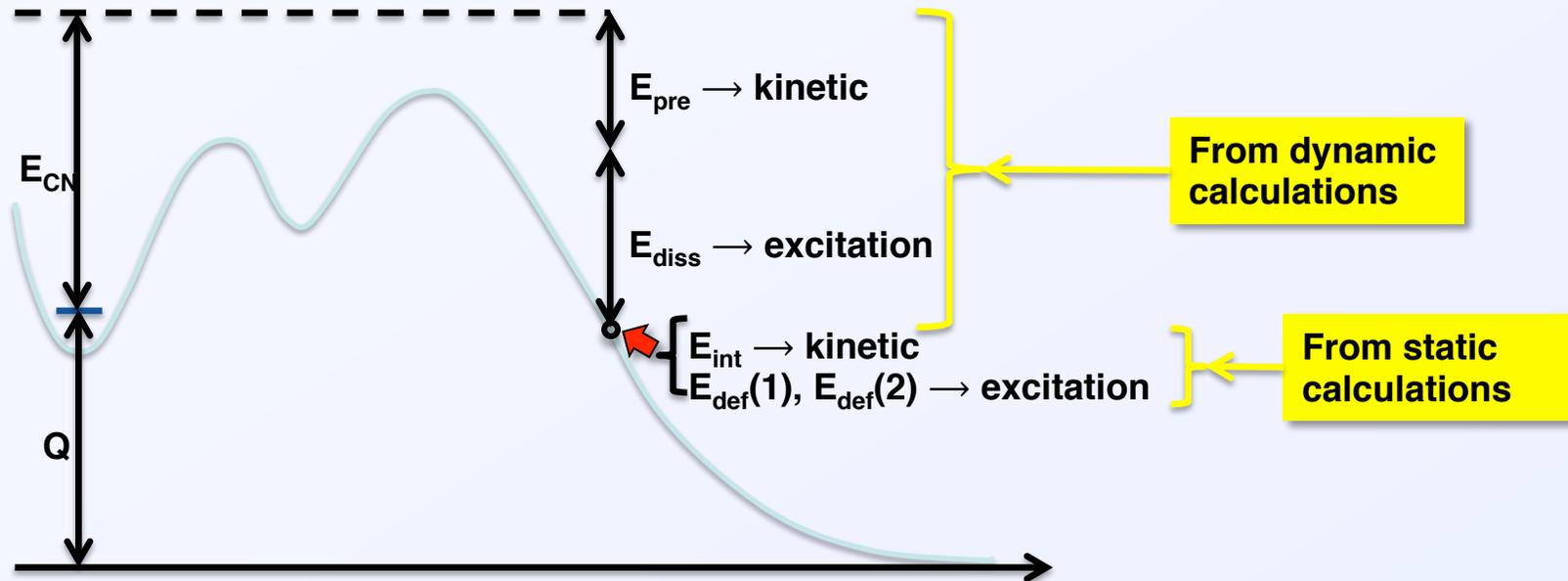


Pre-neutron fission yields for $^{229}\text{Th}(n_{\text{th}},f)$



**Starting from protons, neutrons, and effective interaction:
Results consistent with experiment!**

Calculating fragment energies



- **Static contribution, After quantum localization of pre-fragments:**
 - Identify scission configurations:
 - Integrate energy density for each fragment separately, allow each to relax to its minimum energy, difference gives excitation energy
 - Coulomb energy gives kinetic energy
- **Dynamic contribution (pre-scission energy)**

How do we partition the contribution from dynamics?

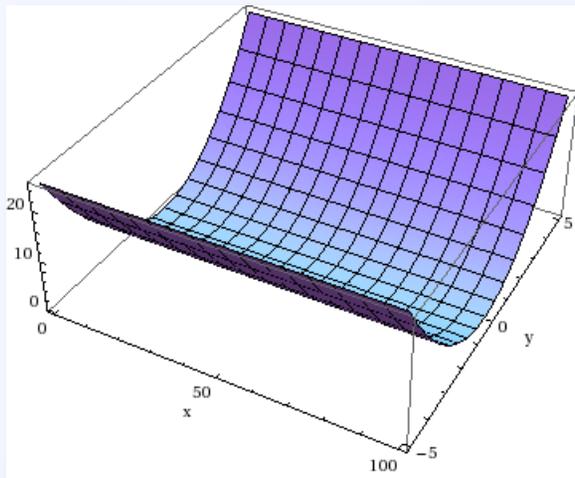
Pre-scission energy: a simplified example

Consider a potential surface

- Flat in x direction
- Parabola in y dir

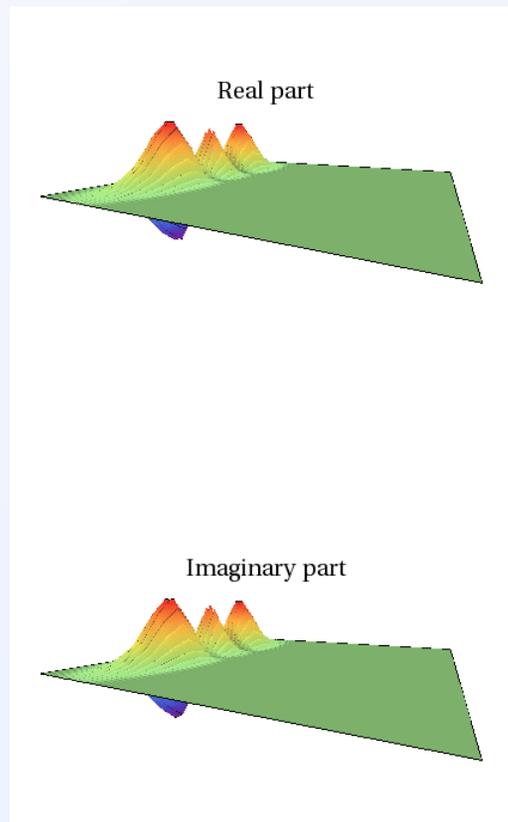
Inertia tensor

- Large in x dir
- Small in y dir
- Zero in x-y

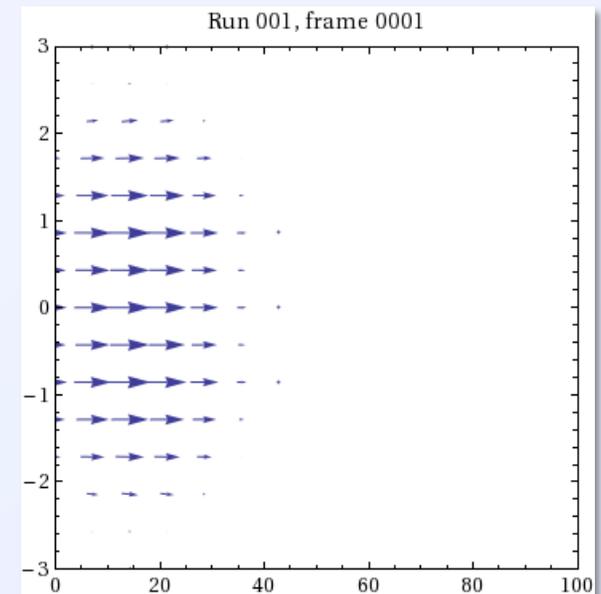


And an initial wave function

- Wave train in x dir
- Harmonic oscillator in y dir

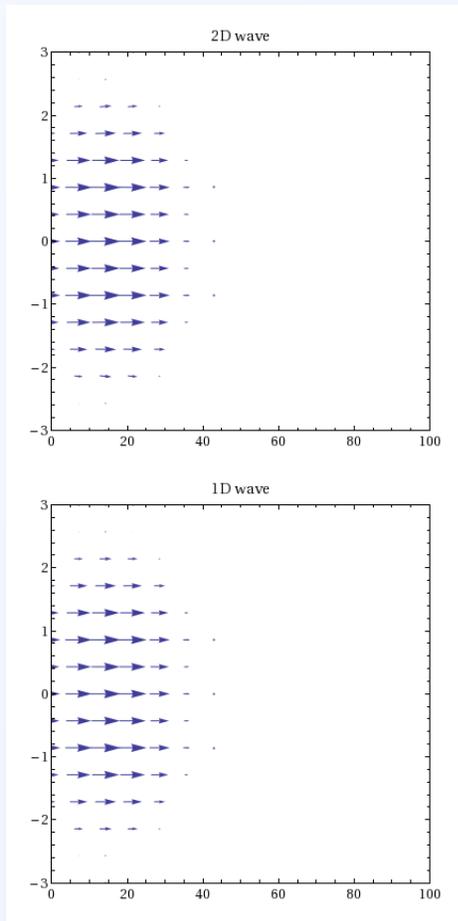


The probability current shows that the motion is not entirely in the x dir!

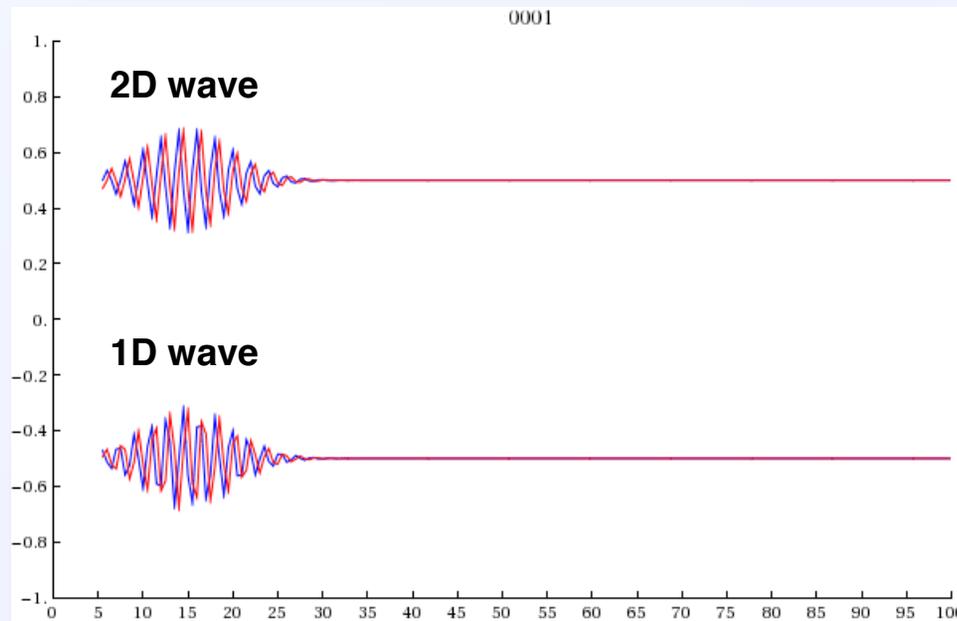


Pre-scission energy: a simplified example

Repeat with same initial form of the wave function with same total energy, inertia tensor nonzero only in x dir \Rightarrow 1D propagation in x dir



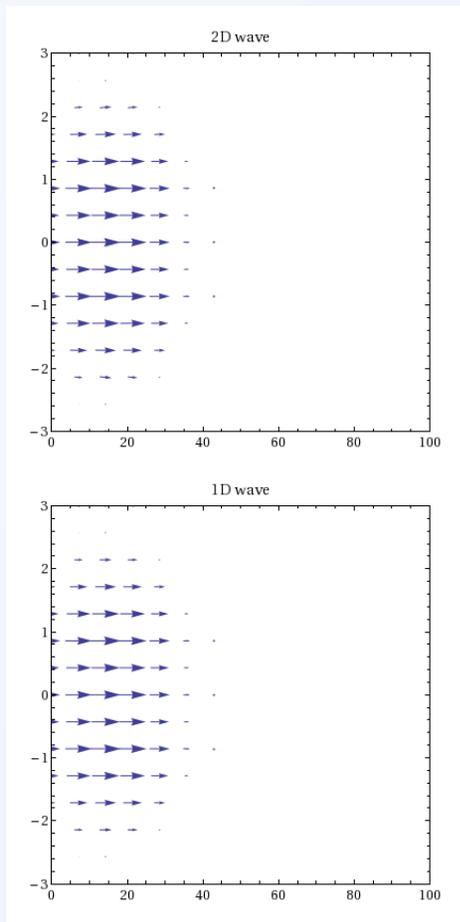
Notice also that the 1D wave is slightly faster:



For fission, we can deduce the pre-scission kinetic energy from the energy difference between 1D and 2D, but how can we find this energy difference?

Pre-scission energy: a simplified example

Repeat with same initial form of the wave function with same total energy, inertia tensor nonzero only in x dir \Rightarrow 1D propagation in x dir



In this simple case, we know (by construction) that

- For 2D wave: $KEx = 4.97$ (in arbitrary units)
- For 1D wave: $KEx = 6.02$ (in arbitrary units)

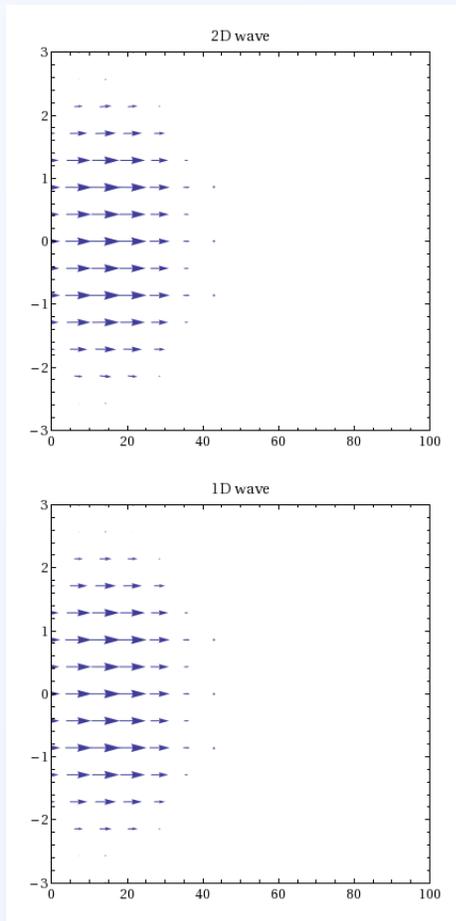
But in the realistic case, how do we find this?

One way is to sit at a point (e.g. $x = 30$, $y = 0$) and measure the flux in the x direction:

- More flux \Rightarrow more kinetic energy

Pre-scission energy: a simplified example

Repeat with same initial form of the wave function with same total energy, inertia tensor nonzero only in x dir \Rightarrow 1D propagation in x dir



In this simple case, we know (by construction) that

- For 2D wave: $KE_x = 4.97$ (in arbitrary units)
- For 1D wave: $KE_x = 6.02$ (in arbitrary units)

But in the realistic case, how do we find this?

One way is to sit at a point (e.g. $x = 30, y = 0$) and measure the flux in the x direction:

- More flux \Rightarrow more kinetic energy

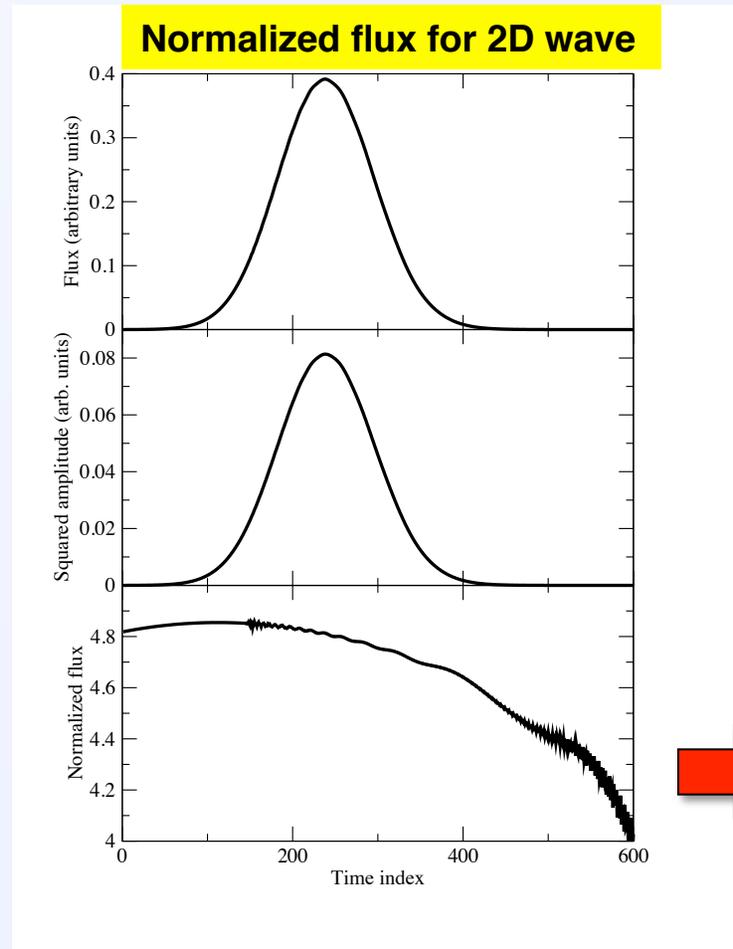
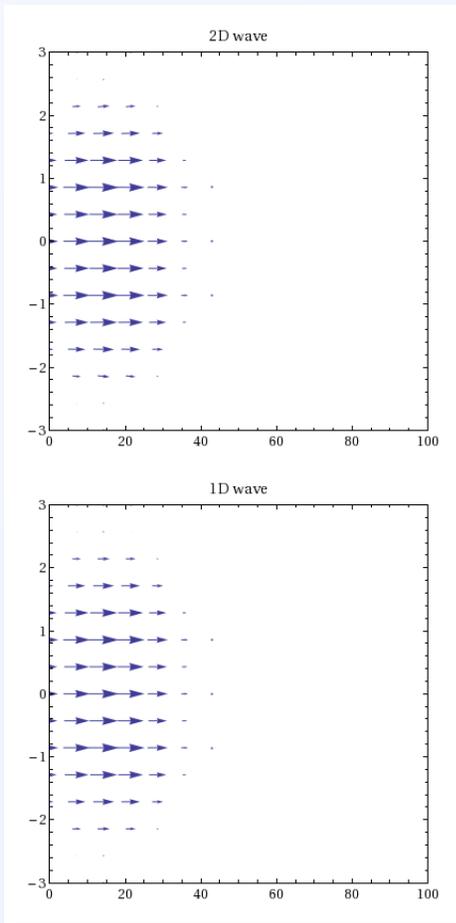
We can even quantify this: if the 2D wave looks like a plane wave in the x direction then

1. We calculate the normalized flux in x dir (flux divided by squared amplitude) at the measurement point
2. This normalized flux is constant in time
3. WKB gives the relation

$$\frac{\text{normalized flux 2D}}{\text{normalized flux 1D}} = \sqrt{\frac{KE_x(2D)}{KE_x(1D)}}$$

Pre-scission energy: a simplified example

Repeat with same initial form of the wave function with same total energy, inertia tensor nonzero only in x dir \Rightarrow 1D propagation in x dir



We deduce: $KE_x = 4.96$
Compare to actual value
= 4.97

Pre-scission energy: the more realistic case

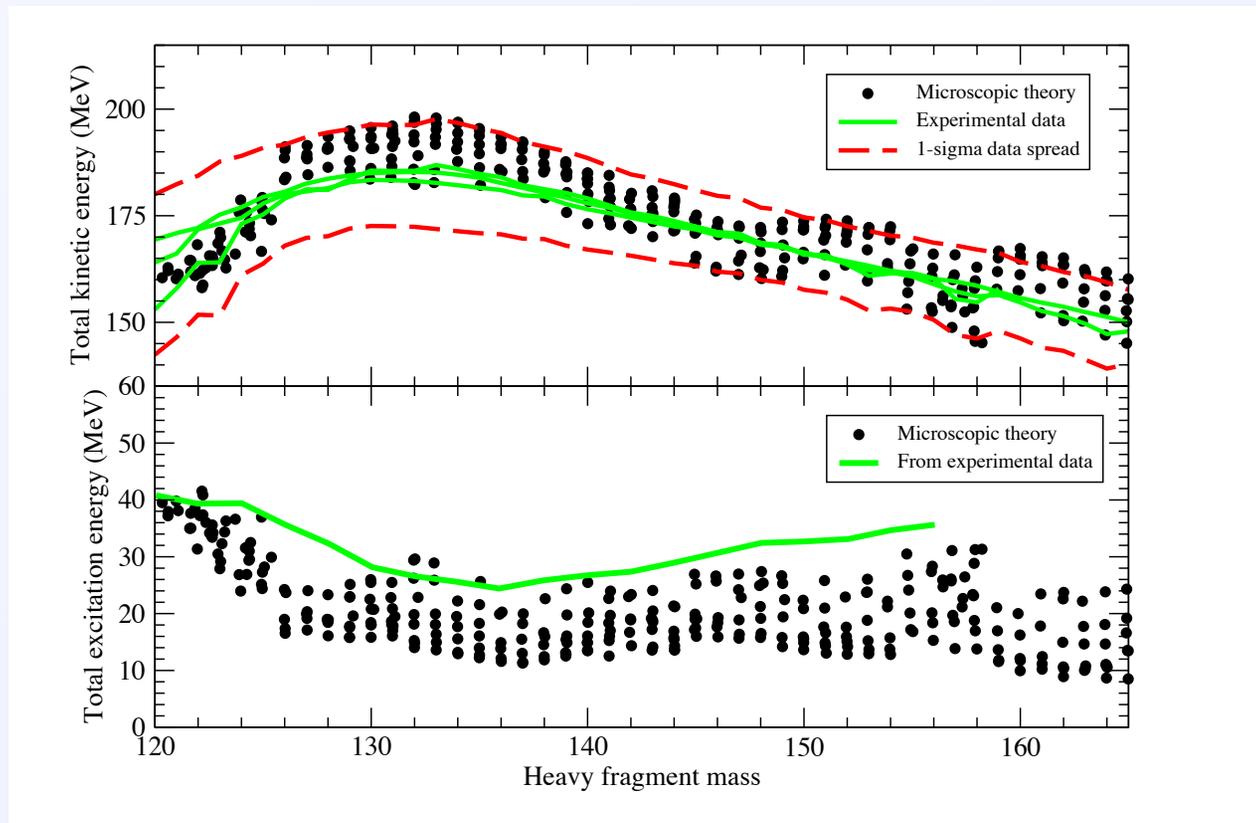
- If we find a state with a normalized flux at a scission point that is constant in time, we can use the approach just described
 - In fission calculations, the x coordinate will be the separation distance between pre-fragments
 - ⇒ We can identify KE_x with the kinetic energy of the pre-fragments at scission (i.e., the pre-scission energy)
 - We invoke energy conservation to say that the remaining energy is transferred to collective modes of the pre-fragments
 - These collective modes are not eigenstates of the final fragments
 - They will evolve in time as the fragments de-excite
 - That de-excitation energy will appear as neutron and γ emission
- We are still missing some physics: More collective & Intrinsic (quasiparticle) d.o.f.
 - For now: excitation energy we calculate is a lower bound
 - Calculations in (d, ξ) for most probable fission in $n_{th} + {}^{239}\text{Pu}$ is consistent with 50/50 split between kinetic and excitation from dynamic contribution



Calculated fragment kinetic and excitation energies for $^{239}\text{Pu}(n_{\text{th}},f)$

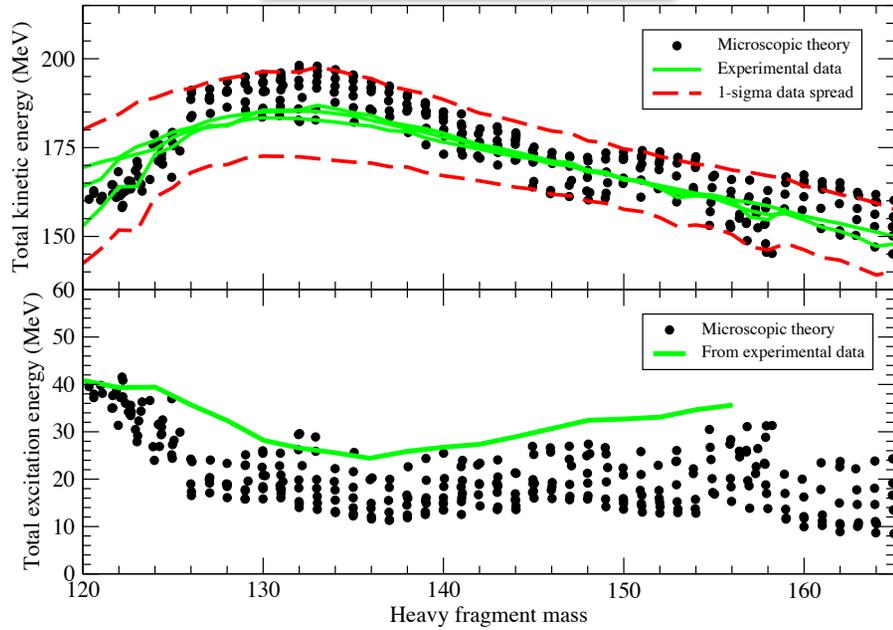
Calculated pre-scission energy due to collective coupling + expected additional few MeV at least from collective-intrinsic (great unknown, see Bernard et al. PRC 84, 044308) \Rightarrow 50/50 split of saddle-to-scission energy between kinetic and excitation is not unreasonable (not too different from estimates by others, e.g. Gönnerwein):

Calculated TKE and TXE using our scission criterion & 50/50 split from dynamic contribution

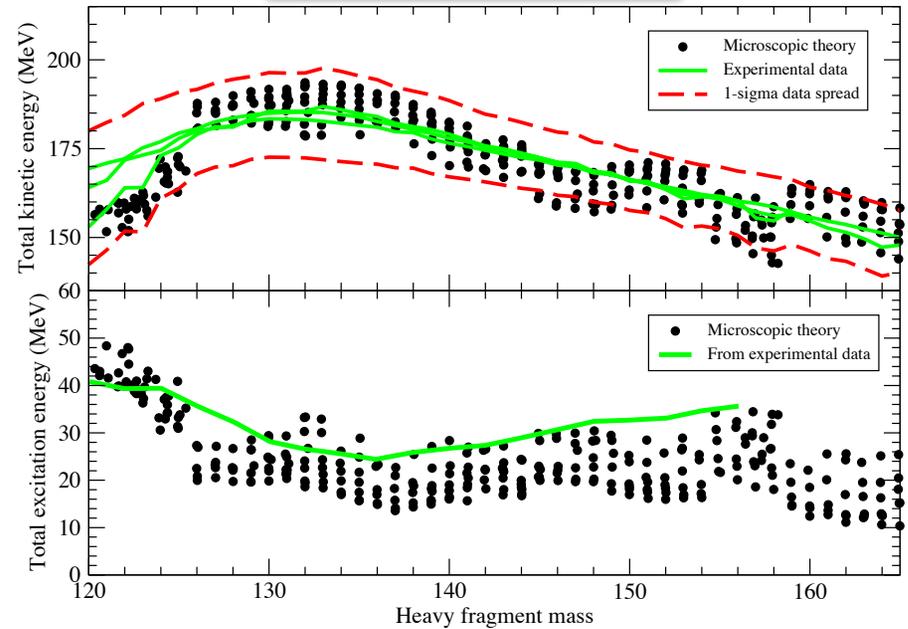


TKE and TXE assuming different split of excitation/kinetic

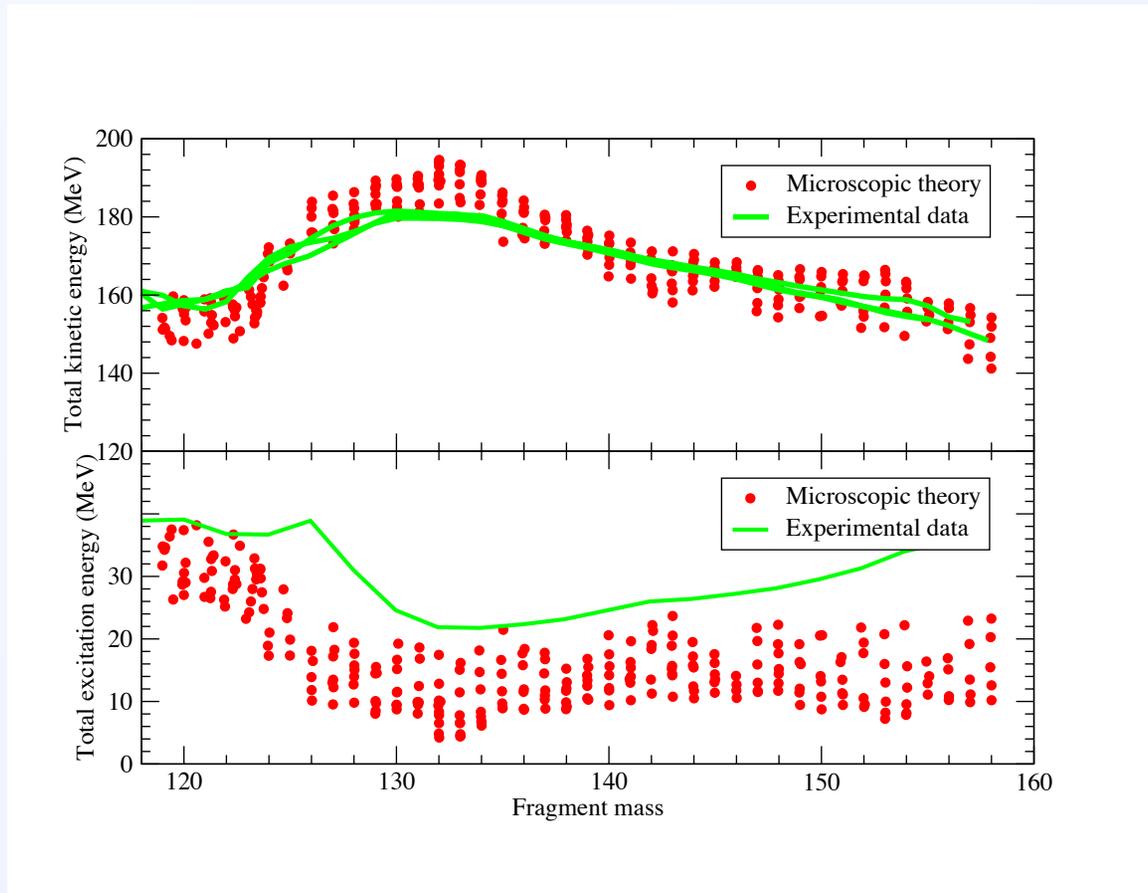
Assuming 50/50 split



Assuming 70/30 split

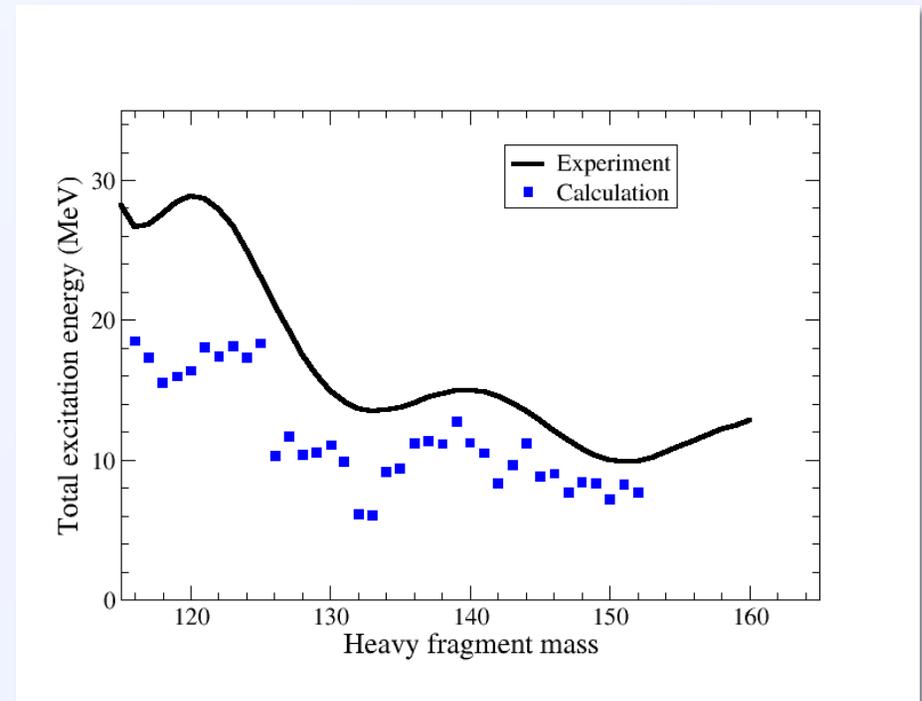
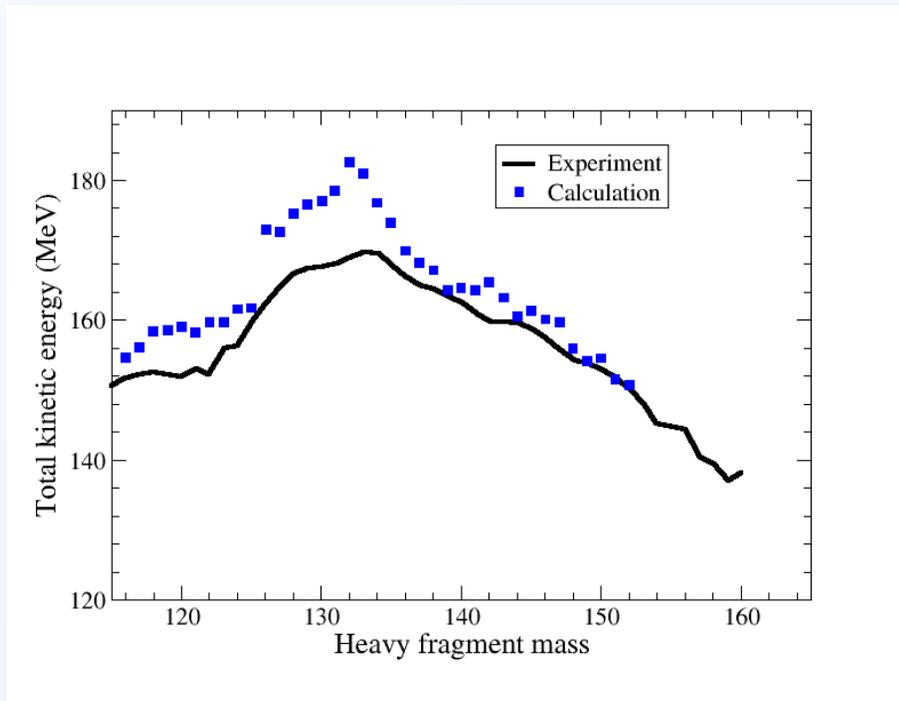


Results for $^{235}\text{U}(n_{\text{th}},f)$: fragment kinetic and excitation energies



**Starting from protons, neutrons, and effective interaction:
Results consistent with experiment!**

Results for $^{229}\text{Th}(n_{\text{th}},f)$: fragment kinetic and excitation energies



**Starting from protons, neutrons, and effective interaction:
Results consistent with experiment!**

Conclusions: summary

- **Ongoing program to develop a microscopic theory of fission, starting from protons, neutrons, and an effective interaction between them**
- **Starting point is mean-field approximation, followed by a hierarchical restoration of correlations beyond the mean field**
- **Progress in understanding scission within a quantum-mechanical framework**
- **Time-dependent formalism gives the dynamics of fission**
- **Today: calculation of multiple fission observables (fragment yields, fragment kinetic and excitation energies,...) within a single, self-consistent framework.**
- **Tomorrow: ?**



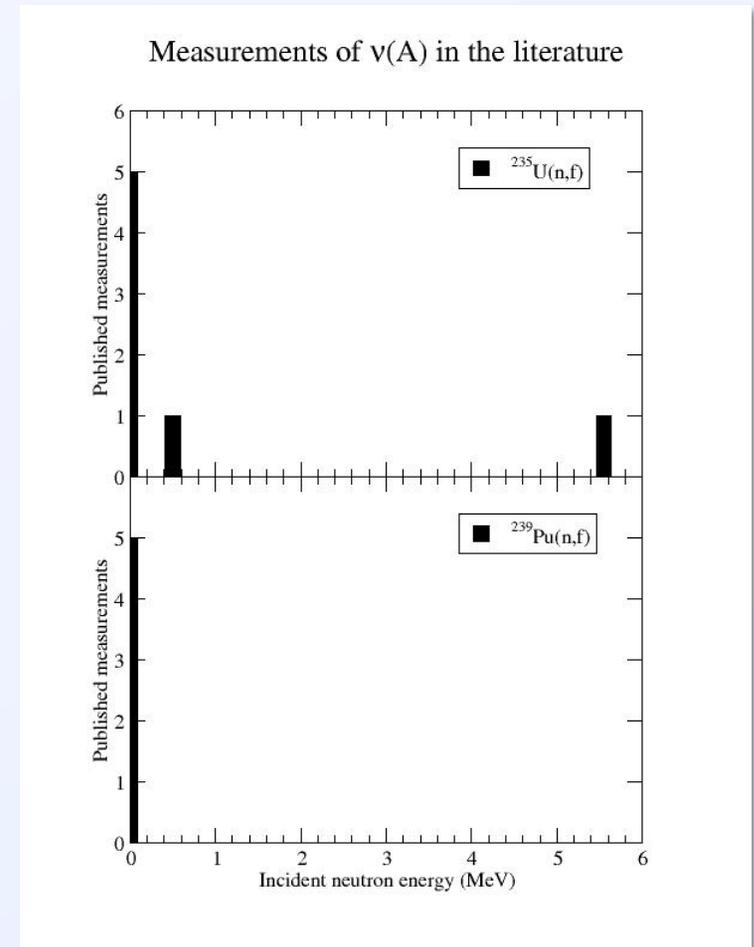
Conclusions: future outlook for theory

- **Current effective interactions contain density-dependent terms**
 - Need to move beyond this to fully non-local interactions
- **What are the appropriate degrees of freedom throughout the fission process?**
 - How do they evolve?
 - Can TDHF help?
- **Calculate coupling between collective and intrinsic d.o.f., and its effect on fission observables**
- **Project wave functions to recover symmetries (e.g., angular momentum, particle number,...)**



Experimental data needs

- **Need multi-parameter measurements, especially as a function of incident energy**
 - **Fragment yields & kinetic energies**
 - **Neutron energies & multiplicities**
 - **Gamma energies & multiplicities**
 - ⇒ **Reconstruct nuclear state at scission**
- **Need measurements that directly probe fission dynamics**
 - **Scission neutrons**
 - **Fission times (with caveats)**
 - **Muon-induced fission**
 - ...



Additional work on microscopic theory of fission

- Scission configurations and their implication in fission-fragment angular momenta (L. Bonneau et al., Phys. Rev. C 75, 064313 (2007))
- Self-consistent calculations of fission barriers in the Fm region (M. Warda et al., Phys. Rev. C 66, 014310 (2002))
- Microscopic description of fission in uranium isotopes with the Gogny energy density functional (R. Rodríguez-Guzmán & L.M. Robledo, Phys. Rev. C 054310 (2014))
- Fission half-lives of superheavy nuclei in a microscopic approach (M. Warda & J. L. Egido, Phys. Rev. C 86, 014322 (2012))
- Microscopic calculation of ^{240}Pu scission with a finite-range effective force (W. Younes & D. Gogny, Phys. Rev. C 80, 054313 (2009))
- Fission barriers at high angular momentum and the ground-state rotational band of the nucleus ^{254}No (J.L. Egido and L.M. Robledo, Phys. Rev. Lett. 85, 1198 (2000))



Additional work on microscopic theory of fission (cont)

- Microscopic study of ^{240}Pu : Mean field and beyond (M. Bender et al., Phys. Rev. C 70, 054304 (2004))
- Microscopic transport theory of nuclear processes (K. Dietrich et al., Nucl. Phys. A832, 249 (2010))
- J. Erler et al., “Fission properties for r-process nuclei”, Phys. Rev. C 85, 025 802 (2012)
- A. Staszczak et al., “Microscopic description of complex nuclear decay: Multimodal fission”, Phys. Rev. C 80, 014309 (2009)
- H. Abusara et al., “Fission barriers in actinides in covariant density functional theory: the role of triaxiality”, Phys. Rev. C 82, 044303 (2010)
- N. Dubray et al., “Structure properties of ^{226}Th and $^{256,258,260}\text{Fm}$ fission fragments: Mean-field analysis with the Gogny force”, Phys. Rev. C77, 014310 (2008)



Useful reviews and books

- J.F. Berger, “La Fission: de la phénoménologie à la théorie”, Ecole Joliot-Curie (2006) (in French)
- H.J. Krappe and K. Pomorski, “Theory of Nuclear Fission”, Lecture Notes in Physics 838 (2012)
- J.F. Berger “Approches de champ moyen et au delà”, Ecole Joliot-Curie (1991) (in French)
- M. Bender et al., “Self-consistent mean-field models for nuclear structure”, Rev. Mod. Phys. 75, 121 (2003)
- E. Moya de Guerra, “The limits of the mean field”, Lecture Notes in Physics 581, 155-194 (2001)
- W. Greiner and J. A. Maruhn, Nuclear Models, Springer (1996)
- J. A. Maruhn, P.-G. Reinhard, E. Suraud, Simple Models of Many-Fermion Systems, Springer (2010)
- P. Ring & P. Schuck, The Nuclear Many-Body Problem, Springer (1980)

